Science Strategy for FTS

Presented to Neutron Advisory Board

Presented by Alan Tennant, Chief Scientist Neutron Sciences Directorate

Director, Shull Wollan Center

June 30, 2016 Clinch River Cabin Oak Ridge, Tennessee

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



Development of science



Strategic Science Plan 2014

Defines key areas for NScD

Ten year Roadmap

<section-header>

Grand Challenges for Neutrons

Workshops on the future

Four workshops on key areas



Future Instrumentation document

Science case for STS

Outlines 3-source strategy

Defines future instrumentation for each source 2015-2016



Update of Strategic Plan 2016

Integrate outcome of workshops

Based on realistic resources

Integrate innovation and partnerships

Five year goals and milestones

Actional Laboratory REACTOR SOURCE

Planning, prioritization, resources



HIGH FLUX ISOTOPE

ational Laboratory REACTOR

NEUTRON

SOURCE

Decision making, monitoring, and budget structure





Quantum Condensed Matter Division

- Magnetic Fields
- Polarization
- Thin films and nanostructures
- Advanced triple-axis spectroscopy
- Theory and modeling
- Diffuse scattering
- Non-equilibrium systems
- High resolution spectroscopy and methods

Sample Environment Group

- Magnetic fields and low temperatures
- High pressure
- Gas handling and high temperature
- Biosoft

Chemistry and **Engineering Division** High pressure Real-time chemistry • • Chemical spectroscopy ٠ Advanced materials and engineering Imaging • Advanced diffraction **Disordered systems** Instrumentation and Methods Group Novel instrumentation and design • Second Target Station • **Moderators** • HFIR cold guide hall planning Polarization

- Optics
- Detectors

Biology and Soft Matter Division

- Soft Matter
- Protein crystallography
- BER engagement
- Deuteration
- Biophysics
- Biohybrid materials

Software, DAS, Modeling

- Data collection, reduction, and analysis
- Computational and resource management CADES
- Science user interfaces
- Materials and data modeling
- Computational science and mathematics



Actions to improve performance

•				
Neutron sources	Staffing	Software and analysis tools	Develop instrument suites	Reform proposal and beam time allocation
HFIR Add 7 th operating cycle SNS Achieve 1.4 MW Utilize D ₂ O	 Build teams across instrument suites (evaluate staff for team roles) Embed postdocs into beamlines and user support Use Technical Professionals (SA) to operate some beamlines (especially for mail-in programs) 	Enable users to do routine analysis and interpretation of data (SANS, QENS, powder inelastic)	 Profiling instruments and suites High throughput instrumentation VENUS RAPID WAND Cold guide optimization at HFIR 	Include broader user communities (dedicate beam time to expand instrument user community to those with faster experiments) User office becomes a proactive recruiter of science communities

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Instrument productivity analysis

2014 publications	No.	Enablers	Possible increase	Difference
BL1a: USANS	0	 Complete instrument commissioning - enter GUP: NIST USANS seems to average about 13 	13	13
BL1b: NOMAD	21	 Rate is increasing - hasn't plateaued yet Reduce background Complete detector complement Profile instrument 	50	29
BL2: BaSiS	20	Jülich hire is critical component	25	5
BL3: SNAP	8	 Dedicated beam time to TOF imaging 	18	10
BL4a: Mag.Refl.	10		20	10
BL4b: Liq.Refl.	9		20	11
BL5: CNCS	23	 Publications have not plateaued yet Dedicate some beam time to soft matter community (hydrogen, QENS) Support soft matter community with postdoc/new staff hire T0 chopper Complete detectors 	40	17
BL6: EQ-SANS	19	 Publications have not plateaued yet 	40	21
BL7: VULCAN	24		24	0
BL8b: RAPID	0	 New instrument for kinetics, parametric, PDF 	50	50
BL9: Corelli	0	Complete commissioning, build up user community	15	15
BL10: VENUS	0	 New dedicated TOF imaging instrument (may reduce SNAP publications when TOF imaging mission migrates to VENUS) 	30	30
BL11a: POWGEN	44	Complete detector upgrade	80	36

Actional Laboratory REACTOR SUBJECT SU



Instrument productivity analysis

2014 publications	No.	Enablers	Possible increase	Difference
BL11b: MANDI	0	 LADI III at year 4 1 publications/10 days of beam time (implies 20/year) 	20	20
BL12: TOPAZ	10	 SXD gets 18–20 Focusing guide Low-temperature goniometer 	20	10
BL13: FNPB	-		-	0
BL14b: HYSPEC	6	 Publication rate has not saturated 	15	9
BL15: NSE	3	• ??	3	0
BL16b: VISION	0	 Completing commissioning (build up user community) Sample changer Postdoc as instrument team member LDRD computational cluster 	40	40
BL17: SEQUOIA	18	Publications have not saturated	20	2
BL18: ARCS	22	 Diversity user community to profile more inelastic power – structural dynamics/thermodynamics – energy materials (e.g., POWGEN user community) Sample changer Mail-in program 	32	10
SNS totals	237		575	338



PEMP notable outcome

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

- Draft plan is circulated within NScD
- 3 year scope
- Goals and milestones
- Implemented with tracking tools
- Comprehensive plan for meeting needs
- Current activities are aligned with this
- Covers training and quality control

Plan to Address Data Needs for HFIR and SNS User Communities

Notable Outcome (BES)

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. (Objective 2.3)

1 Executive Summary

TODO: defining expectations standardization reviews and assessments (internal and external) integrated solutions steering group LDRD neutrons and data shows institutional (ORNL) commitmer Provision of computing resources

2 Defining Needs

Neutron Sciences Directorate (NScD) management has established requirements and standards for data collection, reduction, and analysis software and tools at SNS and HFIR instruments. Requirements and standards were collected by analyzing user satisfaction survey results, direct interaction with users on beam lines, and through a dedicated software forum as part of the SNS HFIR Users Group (SHUG) meeting in October. The SHUG Executive Committee provided a list of recommendations to NScD management.

A working group was formed in October to develop a comprehensive implementation plan towards achieving the standards and requirements outlined above. NSCD management has begun an assessment of every beam line at HFIR and SNS with respect to a typical 'user experience' from setting up the experiment and running a set of measurements to initial data analysis or modeling as required by the instrument type. The assessments and report will be completed by the end of February 2016. This assessment along with the scientific productivity process, and regular review of unplanned operational downtime will form the basis for prioritization and implementation of the data collection, reduction and analysis plan.

A major requirement established is software usability such that a PhD level student should be able to carry out all aspects of a routine experiment from instrument control, sample



Steering group is defining and coordinating actions

Convened in October 2015 by directorate

Technical round sits weekly and every second week full round



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



Wei Tian, HB1A HFIR scientist



Changwoo Do, EQ SANS scientist



Ashfia Huq, Chemical Crystallography Group Lead



Mark Lumsden, TOF Spectroscopy Group Lead

PEMP Timeline – Quarterly reporting

Q	1	

- Convene data and software committee
- Define requirements and standards
- Translate these to a defined checklist

Q2

- Audit our beamlines against requirements and standards checklist
- Liquids Reflectometer back into operation
- Training : external and internal
- Triage NOMAD and MANDI
- Develop planning for PEMP with strategic science plan

- Q3 Introduce software evaluation via
- evaluation via external instrument reviews
- Embed software scientists
- LDRD investment into software and modeling
- Put in place monitoring and collecting feedback
- HFIR IPTS
 integration
- scientific user interface challenges
- Triage HFIR SANS
- Review our plans and progress

Q4

- Triage IMAGING
- Tracking for quality control and user debriefs around checklist
- R2A2s & EPMs that match the requirements
- Launch Instrument documentation project
- PEMP plan
 completion

OAK RIDGE HIGH FLUX SPALLATION National Laboratory REACTOR SOURCE

Strategy for data collection, reduction, and analysis

- Provide integrated data lifecycle management (DOE and NSF compliant)
- Standardization of DAS, data, and reduction/analysis applications and their integration based on EPICS, ICAT, and MANTID
- Management to defined data and software standards and requirements
- Institutionalize data and metadata capture/recording
- Provide and support a comprehensive and powerful data analysis and visualization environment
- Facilitate community contributions and partnerships
- Team based approach with embedding of software scientists and training
- Utilize extensively science user interfaces and automation
- Provide leadership level data and computational capabilities
- Priorities and solutions deployed to maximize science impact and productivity
- Advocacy and stewardship of neutron science needs
- Review, quality assurance, and customer satisfaction to ensure effectiveness



Standards and requirements

- Acceptable pre-experiment planning support
- Documented instructions at PhD student level to operate the instrument for routine cases
- Include standard operation of common sample environments (change temperature, field etc.)
- Documented instructions at PhD student level on data access, reduction, and analysis it is a requirement that the calibration and reduction algorithms and procedures are checked and clearly documented
- Commands and controls at a level that allows trained user to operate instrument with occasional expert phone support
- Acceptable data access and automation i.e. not time consuming, self explanatory, efficient, accurate
- Accepted training process
- Named instrument contact capable of providing expert support during and post experiment
- Accountability and review of our meeting of requirements
- Quality control and assurance
 walk rounds and debriefings, user feedback, accountability and review, embedding of NDAV software scientist with instrument teams to support instrument scientists in their activities
- Guarantee of accurately reduced and visualizable data that allows user to understand their measurement quality and determine informed choices for optimal outcomes of experiment
- · Wide adoption of standardization and commonality
- Integrated data archiving and access that works seamlessly with IPTS giving a unified user experience
- Assurance that users leave with correctly reduced data, access to it, and the ability to undertake standard analysis

Working group, user feedback, and SHUG software breakout



Audit beamlines

- Audit beamlines against requirements and standards list
- Conducted January and February 2016
- Report received March 2016
 Audit Teams

	SNS	HFIR	Team Lead	Subject matter expert	Group Leader/designee	Post Doc/Student/IS
Inelastic	ARCS		Garrett Granroth	Luke Daemen	Timmy Ramirez	Alex Thaler
	CNCS		Garrett Granroth	Luke Daemen	Timmy Ramirez	Alice Taylor
	SEQUOIA		Garrett Granroth	Dan Pajerowski	Timmy Ramirez	Alex Thaler
	HYSPEC		Garrett Granroth	Dan Pajerowski	Timmy Ramirez	Alice Taylor
	BASIS		Garrett Granroth	Doug Abernathy	Jaime-F-Baca	Rana Ashkar
	VISION		Garrett Granroth	Doug Abernathy	Jaime-F-Baca	Panchao Yin
		HB1: PTAX	Garrett Granroth	Andre Savici	Mark Lumsden	Travis Williams
		HB1A: FIE-TAX	Garrett Granroth	Andre Savici	Mark Lumsden	Travis Williams
		HB3: TAX	Garrett Granroth	Andre Savici	Mark Lumsden	Travis Williams
		CG-4C: CTAX	Garrett Granroth	Andre Savici	Mark Lumsden	Travis Williams
Diffraction	POWGEN		Thomas Proffen	Ovi Garlea	Matthew Tucker	Daniel Olds
	NOMAD		Thomas Proffen	Ovi Garlea	Matthew Tucker	Daniel Olds
	SNAP		Thomas Proffen	Matthias Frontzek	Matthew Tucker	Shanmin Wang
	TOPAZ		Thomas Proffen	Matthew Cuneo	Bryan Chakoumakos	Timothy Prisk*
	MANDI		Thomas Proffen	Ovi Garlea	Bryan Chakoumakos	Brad O'Dell
	CORELLI		Thomas Proffen	Matthias Frontzek	Ashfia Huq	Matthew Cuneo/Timothy Prisk*
		HB-2A	Thomas Proffen	Matthias Frontzek	Ashfia Huq	Daniel Olds
		IMAGINE	Thomas Proffen	Matthew Cuneo	Bryan Chakoumakos	Timothy Prisk*
		HB-3A	Thomas Proffen	Matthew Cuneo	Ashfia Huq	Timothy Prisk*
Other	U-SANS		William Heller	Changwoo Do	Greg Smith	Zhe Wang
SANS	EQ-SANS		Richard Ibberson	Qian Shuo	Timmy Ramirez-Cuesta	Panchao Yin
REFL	LR		William Heller	Timothy Charlton	Mike Fitzsimmons	Rana Ashkar
Engineering	MR		William Heller	Timothy Charlton	Greg Smith	Rana Ashkar
	VULCAN		William Heller	Tom Watkins*	Andrew Payzant	Jeff Bunn
	SPIN ECHO		William Heller	Georg Ehlers	Mike Fitzsimmons	Zhe Zhang
		Bio-SANS	William Heller	Changwoo Do	Andrew Payzant	Zhe Zhang
		GP-SANS	William Heller	Changwoo Do	Mike Fitzsimmons	Zhe Zhang
		HB-2B	William Heller	Tom Watkins*	Ke An	Indu Dhiman
		Imaging	William Heller	Charles Finney*	Andrew Payzant	Jeff Bunn
* - non-NScD	personnel					



Richard Ibberson, Chaired Beamline Audit

nal Laboratory | REACTOR

Integration of teams from DAS, data, and analysis/visualization

Teams are now tasked to work together to provide integrated solutions



Garrett Granroth, Scientific Data Analysis Group Lead



Shelly Ren, Science Information Systems Team Lead



Steve Hartman, Data Acquisition Group Lead

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Embedded software scientists on beamlines

NDAV Staff		Instrur	nent(s)	
Ricardo Leal	BioSANS	GPSANS	Imagine	
Mathieu Doucet	EQSANS	uSANS	RefL	
Peter Peterson	Nomad	PowGen	SNAP	
Wenduo Zhou	Vulcan	HB-2B	HB-2A	HB-3A
Vickie Lynch	Topaz	Mandi		
Ross Whitfield	Corelli	WAND		
Garrett Granroth	HB-1A	HB-1	HB-3	CTAX
Steve Hahn	RefM			
Jean Bilheux	Imaging			
Andrei Savici	HYSPEC	CNCS		
Jiao Lin	ARCS	SEQUOIA		
Jose Borreguero	Basis			
Stuart Campbell	Vision			

Science User Interface - Liquids Reflectometer

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Technical Achievement

The SNS Liquids Reflectometer has been upgraded to an EPICS-based data acquisition system, incorporating instrument and sample-environment control (e.g. Langmuir trough, below) in a selfguided, yet powerful user interface (UI). Data auto reduction is integrated creating a Science Environment.



16 Neutron Advisory Board June 30, 2016

Integrated data lifecycle management – proposal, experiment, reduction, publication



Effective partnership with computational science, mathematics, and theory

Present

Center for Accelerating Materials Modeling (CAMM) funded by BES MSED, linking neutron scattering (SNS data) and materials simulations

Accurate quantified mathematical methods for neutron science (ACUMEN) funded by ASCR, developing innovative methods focused on core mathematical challenges relevant to neutron scattering

Adaptive biological imaging (ABI) and Biofuels science focus area (SFA) funded by BER

> http://camm.ornl.gov http://cam.ornl.gov/acumen

Future

Workshop on Frontiers in Data, Simulation, and Modeling, March 2015

Exascale Computing Project (ECP): A full proposal invited for multiscale software environment for soft materials innovation; partnered with CAMERA, ACUMEN, and EQUINOX; planning for co-design proposal

FY17 LDRD focus area: Next-generation data, modeling, and simulation for neutron science

Virtual Theory Group @ Shull Wollan Center headed by Prof Christian Batista



Actional Laboratory REACTOR SUBJECT SPALLATION NEUTRON SOURCE

Partnership with high performance computing and mathematics focusing on deployable applications/solutions



* **Bao**, et. al, 'Hierarchical Optimization for Neutron Scattering Problems', in Review JCP, 2016.



ACUMEN



* **Archibald**, **et. al**, 'Image Reconstruction from Undersampled Fourier Data', JSC, 2015.

Accurate Quantified Mathematical Methods for Neutron Science

Provide leadership level data and computational capabilities



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Accurate Quantified Mathematical Methods for Neutron Science

Maximizing science impact and productivity



NEUTRON

SOURCE

National Laboratory REACTOR

Discussion





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Transition from Instrument User Interfaces to Scientific User Interfaces

<u>م</u>					CS-Studio (on bl4b-daq1.sns.gov)	
<u>F</u> ile Edit Se <u>a</u> rch <u>R</u>	un <u>C</u> S-Studio Windo	w Help				
💼 🔛 🖌 🙀 🕫	1 1 1 1 A -					
🖉 Proposal/Operating	Mode 🕴 🚂 Langmuir	🚝 Dashboard				
	Liquids F	Reflectomete	r User Experime	nt		
	Elquius I					
1. Proposal/Operat	ing Mode 2. Prepare	for Direct Beam 3. C	Collect Direct Beam 4. Align	5. Collect Data	Dashboard	
1.1 Proposa	l Information					
Proposal #:	IPTS-17174	Switch				
Proposal Title:	Self-assembly behavior	of amphiphilic nanocages a	at liquid-air interface			
Team Members:	Candice Halbert:CEH	:E;Jim Browning:JFB:E;Pa	nchao Yin:YINPANCHAO:P	(Name:XCAMS/UCAMS:Role, where 'P' indic Primary Investigator, 'E' is Editor, and 'V' is	ates Viewer.)	
Run Cycle:	SNS 2016-A					
1.2 Sample I	Environment D	evice and Opera	ting Mode			
○ NO Special SE [Devices					
ORobot						
O Liquid/Solid Cel	I					
OElectrochemica	al Cell					
ORheometer						
Multi-Environm	ent Chamber	C Free Liquid	~			
Elow/Shear Cell	jn I	Unee Liquid -	23			
1 7 Align con	malo REEORE c	allocting direct	hoom data?			
	IIIPIE BEFORE C	onecting unect	beam uatar			
Substrate thick	ness: 20.00 mm					
Change Mode O	only: Reflect	ivity Direc	t Beam			
Inst	rument Status			Selected Proposal:	IPTS- 17174	
CI	hoppers Phase Locked	ок	Busy?	Selected SE Device:	Langmuir Trough	
M	otors Status	•	×	Selected Operating Mode	: Free Liquid	
50	perating Mode	Eree Liquid	Operating Status Is the instrument busy?	Liquid 50mm 3.5 0.3	© Reset	
м	otor Positions	0 (0: Sample; 1: I	Dk Green: NO Direct B Orange: YES		Next	

- Software Upgrade of the Liquids Reflectometer at SNS.
- All instrument control and data reduction software upgraded.
- Design of a scientific user interface to guide users through the steps of an experiment.

