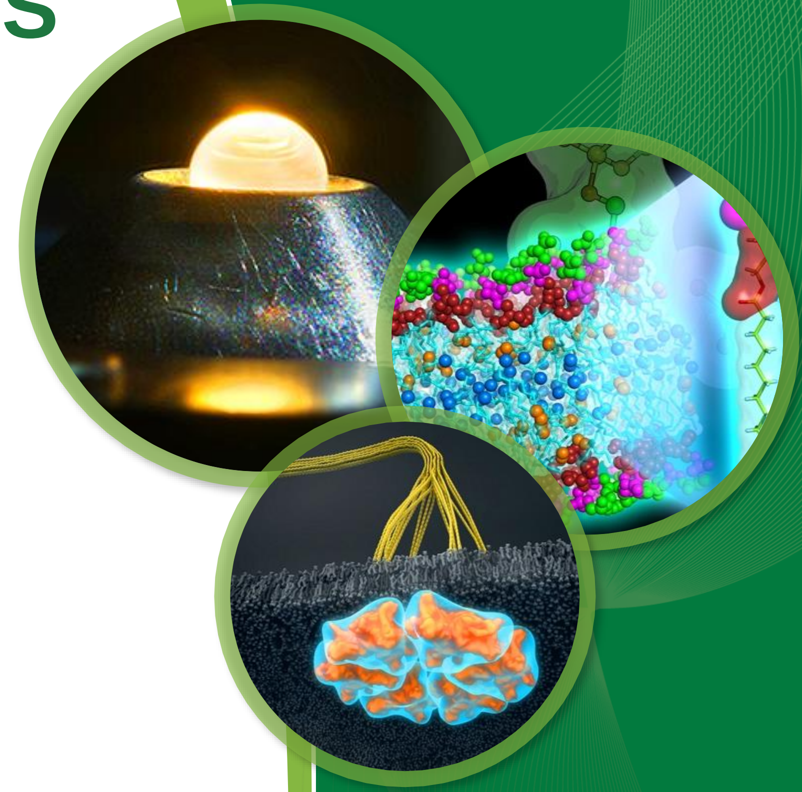
Science Strategy for FTS



Presented to
Neutron Advisory Board

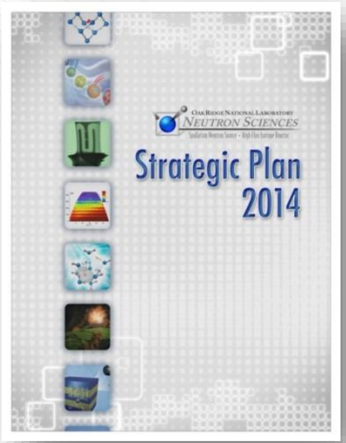
Presented by
Alan Tennant, Chief Scientist
Neutron Sciences Directorate

Director, Shull Wollan Center

June 30, 2016
Clinch River Cabin
Oak Ridge, Tennessee

Development of science

September 2013

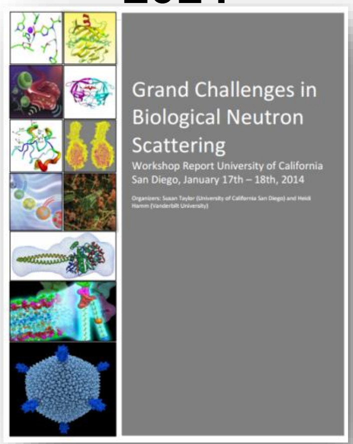


Strategic Science Plan 2014

Defines key areas for NScD

Ten year Roadmap

August 2014

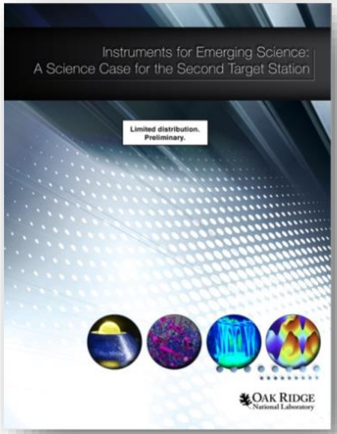


Grand Challenges for Neutrons

Workshops on the future

Four workshops on key areas

October 2014



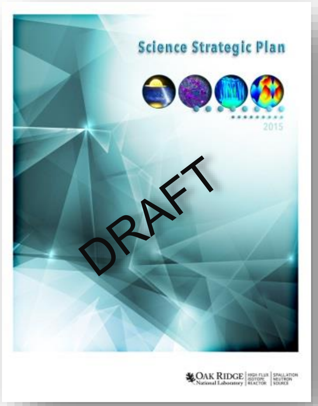
Future Instrumentation document

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

Planning, prioritization, resources

Divisions and Groups

Develop proposed plans

Cross-cutting working groups

Assess weaknesses and potential

Develop integrated targets, goals, and resourcing

Directorate and divisions

Integrated planning, budgeting, and decision making

Inputs

Instrument productivity reports from instrument scientists and users

Strategic science drivers

Workshop reports

Outputs

Profile

Priorities

Engagement

Funding and resources

Productivity

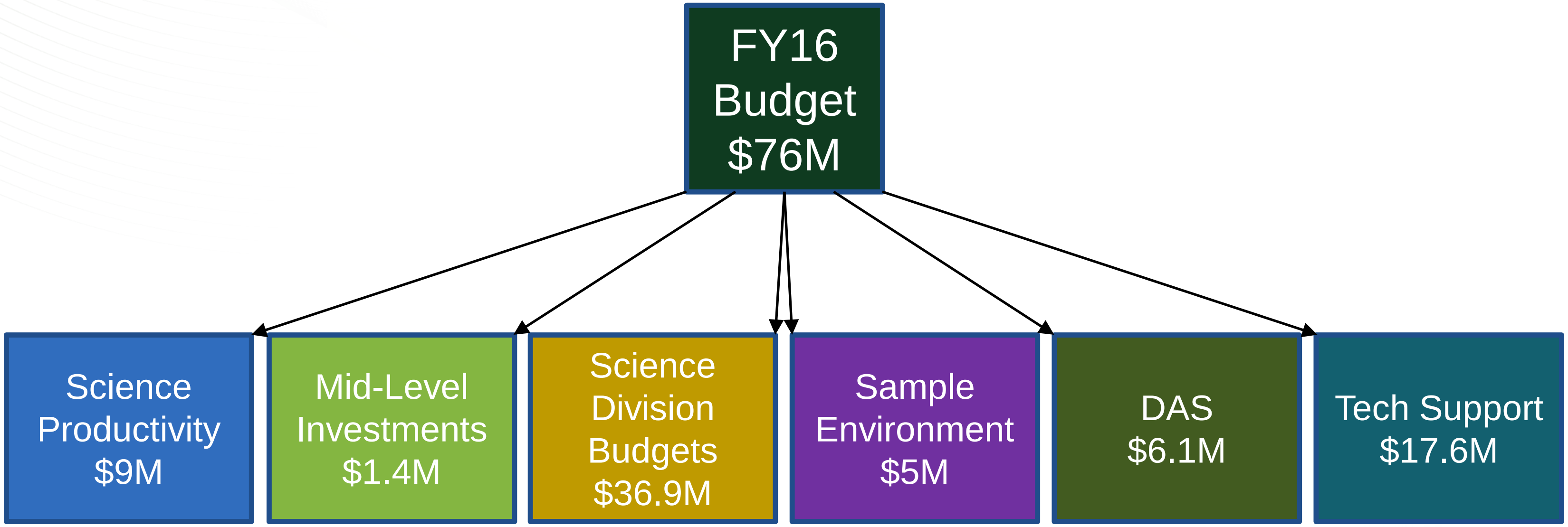
Impact

Staff/program development

Outcomes in strategic planning tool

Successfully cross linked facility planning.

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
- 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

- **Performance, Project Management, and Review**
- **Ambition to double publications from 2014**

Neutron sources	Staffing	Software and analysis tools	Develop instrument suites	Reform proposal and beam time allocation
HFIR Add 7th operating cycle **SNS** Achieve 1.4 MW Utilize D_2O	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

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

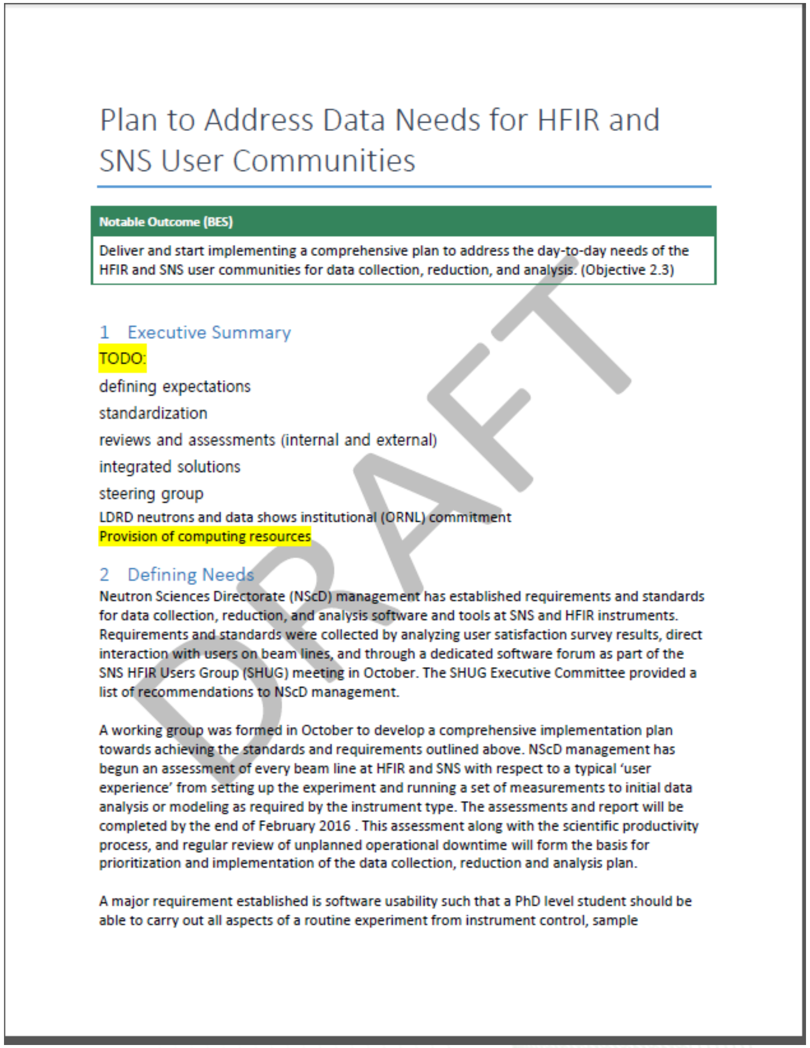
Instrument productivity analysis

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) commitment

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

DRAFT

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Steering group is defining and coordinating actions

Convened in October 2015 by directorate

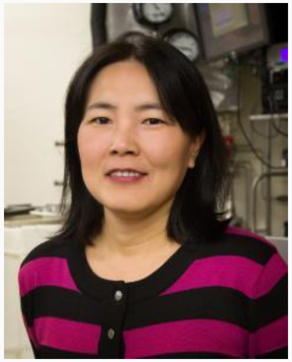
Technical round sits weekly and every second week full round


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

Q1

- 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 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

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

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

Teams are now tasked to work together to provide integrated solutions

Embedded software scientists on beamlines

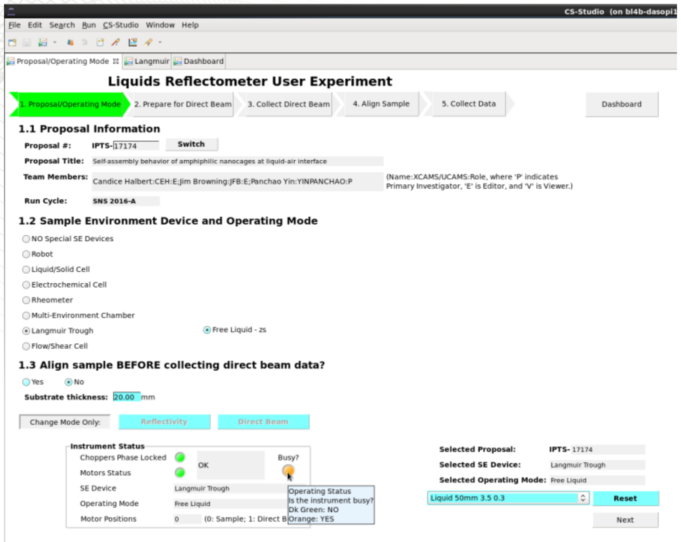
NDAV Staff	Instrument(s)			
Ricardo Leal	BioSANS	GPSANS	Imagine	
Mathieu Doucet	EQSANS	uSANS	RefL	
Peter Peterson	Nomad	PowGen	SNAP	
Wenduo Zhou	Vulcan	HB-2B	HB-2A	HB-3A
Vickie Lynch	Topaz	Mandi		
Ross Whitfield	Corelli	WAND		
Garrett Granroth	HB-1A	HB-1	HB-3	CTAX
Steve Hahn	RefM			
Jean Bilheux	Imaging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

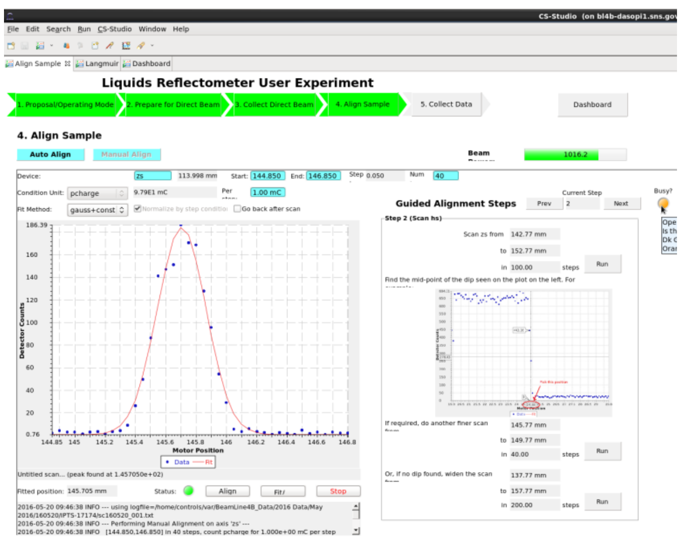
Garrett Granroth,
Scientific Data Analysis
Group Lead

Shelly Ren,
Science Information Systems
Team Lead

Steve Hartman,
Data Acquisition
Group Lead

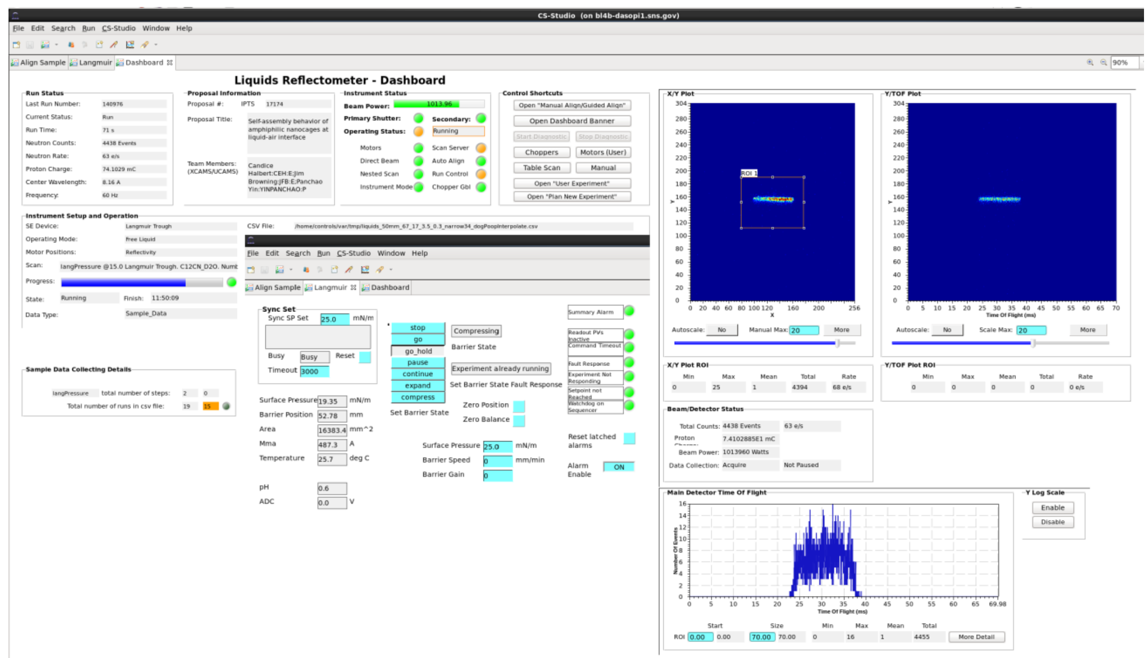
Science User Interface - Liquids Reflectometer





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 self-guided, yet powerful user interface (UI). Data auto reduction is integrated creating a Science Environment.



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

OAK RIDGE National Laboratory

GUEST PORTAL HOME FEEDBACK? ABOUT ORNL CONTACT US

MY ACCOUNT

- Emergency Contacts
- View Profile
- Admin Options

PROPOSALS

- Confirmed 1
- Completed 8
- Create a Proposal
- Proposal System (Neutron Sciences)

MY RESEARCH

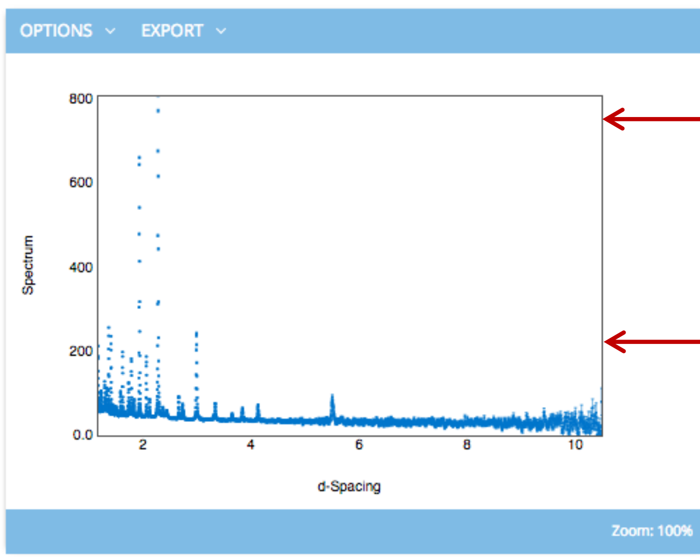
- Access Experiment Data
- Shipping Research Samples to ORNL
- Register Publication

FOR VISITORS

Completed Proposals

ID	Title	Beamline	Experiment Dates	Team
15209	Settling a Scientific Debate by Investigating the Structure-Property Relationships of Disordered Aurivillius Phases	POWGEN	12-MAY-16 to 14-MAY-16 Results	M.Dolgos T.Surta

Run title	Ca Ramping up
Run start	May 13, 2016, 5:27 a.m.
Run end	May 13, 2016, 6:27 a.m.
Duration	3601.1 sec
Total counts	9.59123e+06
Proton charge	3.76114e+12



POWGEN
IPTS-15209, Run 28167

- **Allows users to further explore their data during the experiment**
- **Now they can zoom in on weak Bragg peaks from any web enabled device**

SPALLATION NEUTRON SOURCE

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

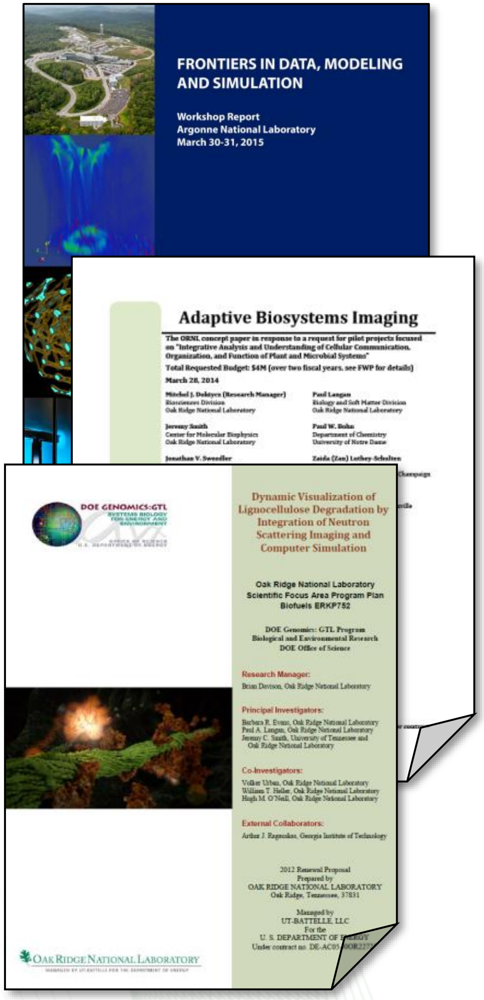
Future

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



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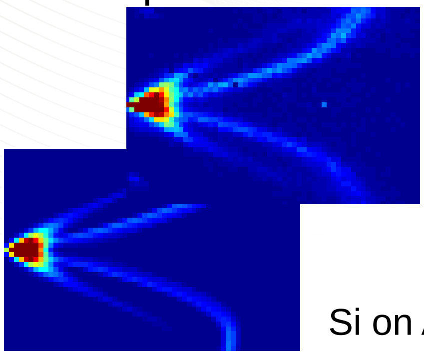
Partnership with high performance computing and mathematics focusing on deployable applications/solutions

Science and data

Mathematics and algorithms

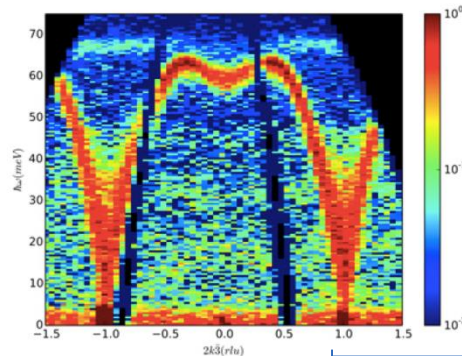
Computational implementation on architecture

Inelastic dispersion fitting for phonons

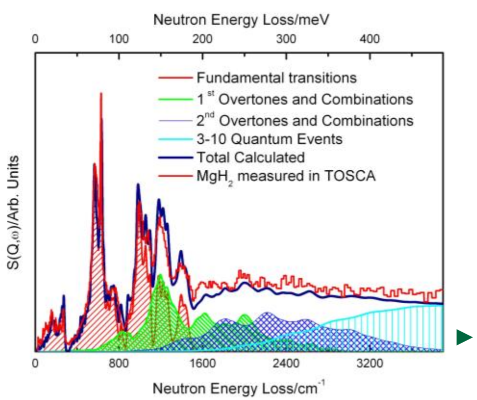


Si on ARCS

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



Uncertainty Quantification mathematics built in to McStas to model resolution functions



Resolution at high energies is low for spectrum *(eg. MgH_2)*. Using Bayesian analysis on the raw data to provide best mean estimate and uncertainty at high energies of spectrum.

UQ applied to chemical spectrum analysis

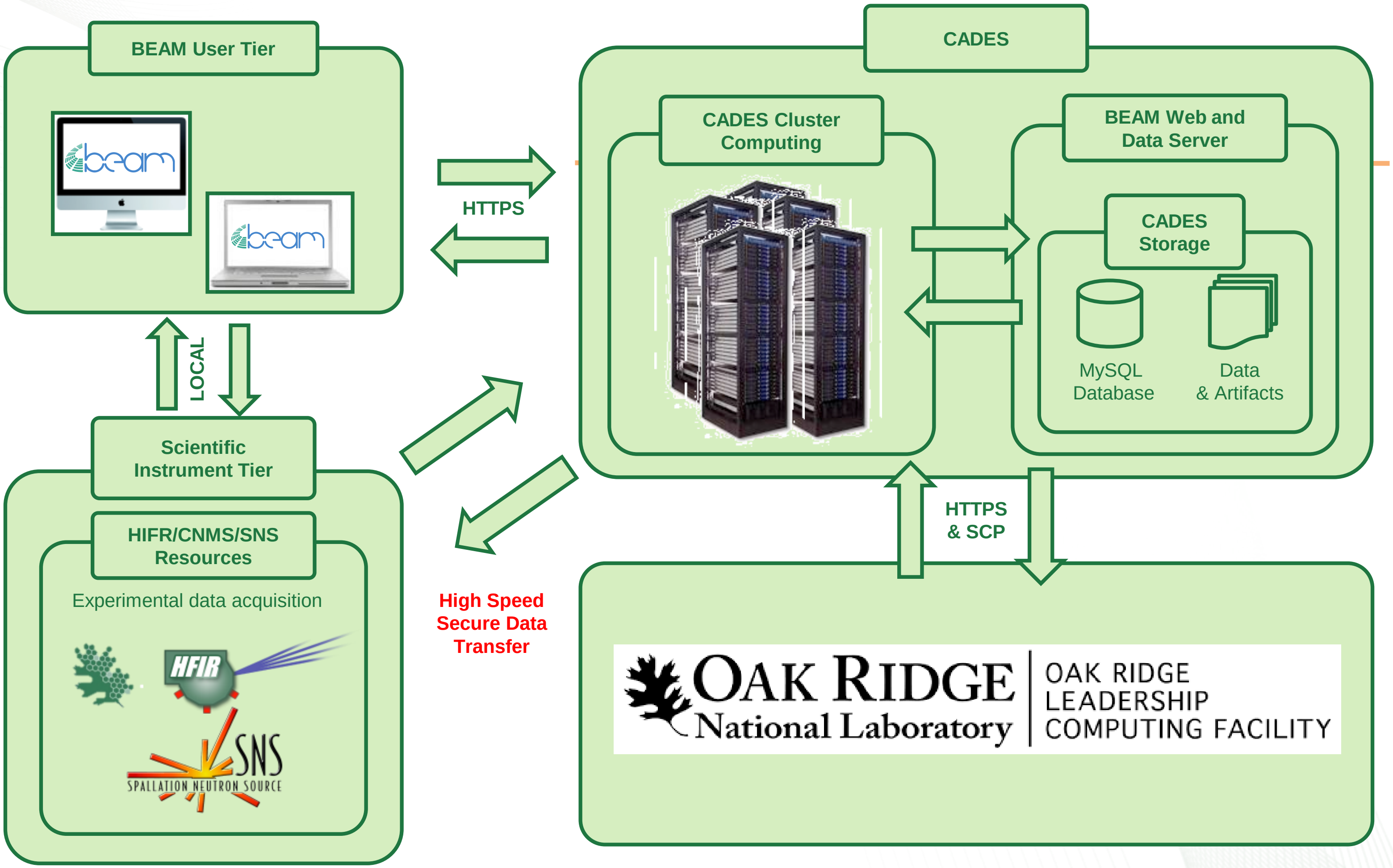
High fidelity fast tomography

Rendering reduced from 6hrs to minutes

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

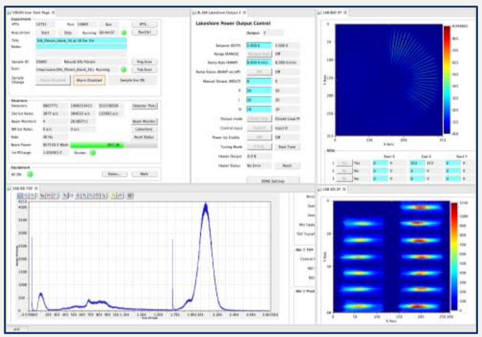
ACUMEN Accurate Quantified Mathematical Methods for Neutron Science

Provide leadership level data and computational capabilities



Maximizing science impact and productivity

Data acquisition Instrument control

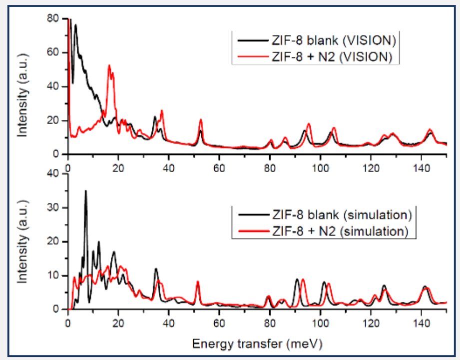


CSS control system studio

ADARA

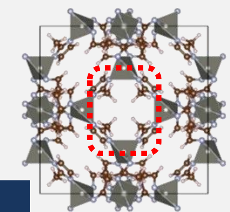
EPICS

Automatic Data Reduction

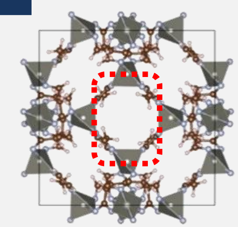


MANTID

Data Analysis & Materials Modeling



VirtuES Cluster



ACUMEN

CADES Compute & Data Environment for Science

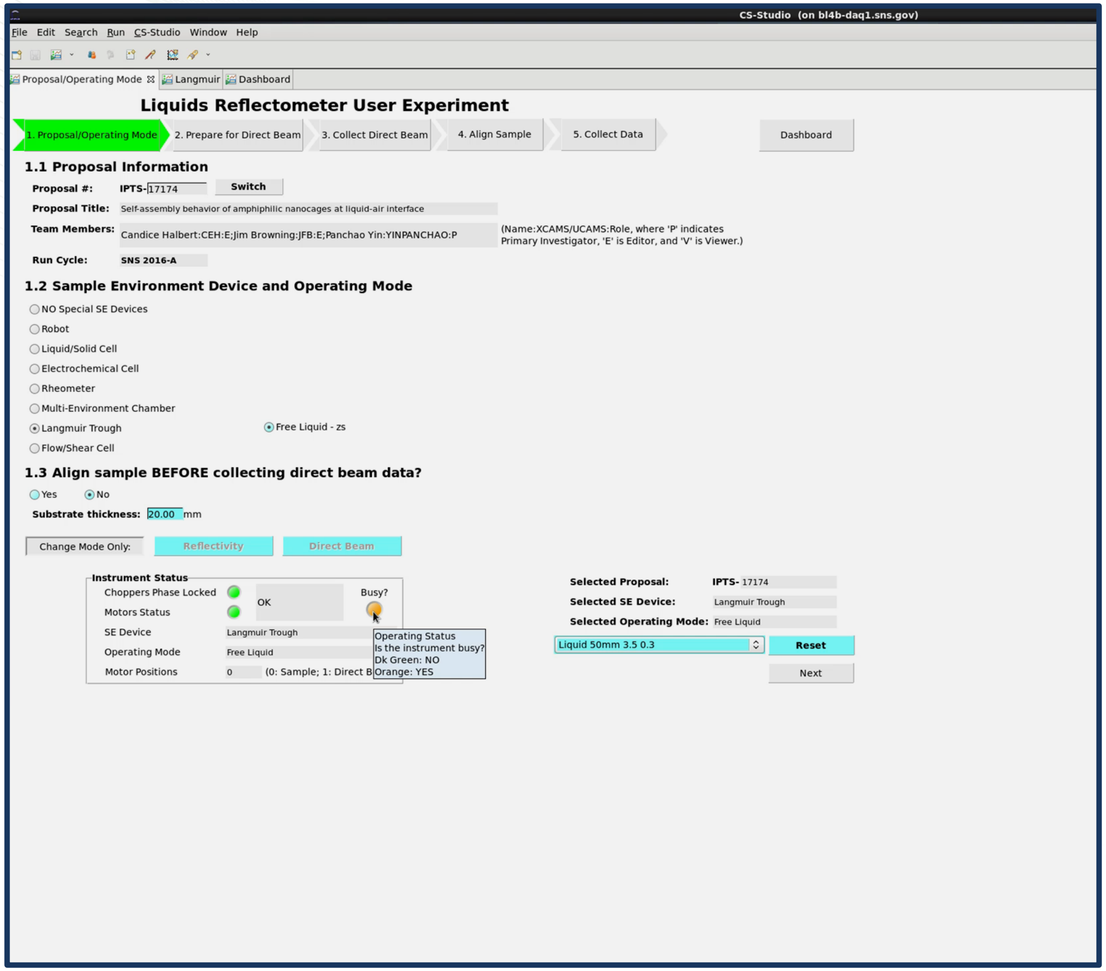
Experiment steering
Human or automatic

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

Discussion

Transition from *Instrument User Interfaces* to *Scientific User Interfaces*



- 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.