Update on Neutron Sciences at ORNL

Presented to

SNS Accelerator Advisory Committee

Presented by

Paul Langan
Associate Laboratory Director
Neutron Sciences

March 24, 2015

BES investment has created 2 advanced neutron scattering user facilities

High Flux Isotope Reactor (HFIR)
Intense steady-state neutron flux and a high-brightness cold neutron source

Spallation Neutron Source (SNS)
World's most powerful accelerator-based neutron source

U.S. Department of Energy user facilities:
Unique capabilities available through peer review

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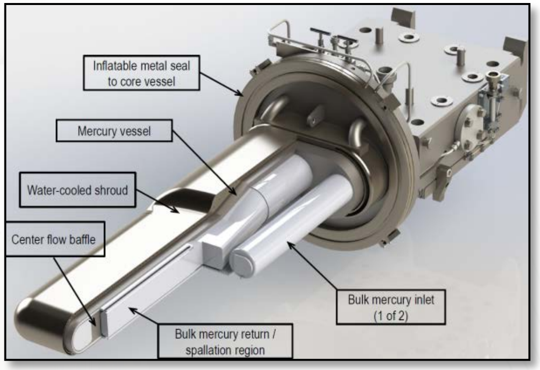
SNS and HFIR met all goals in Fiscal Year 2014

HFIR

- Delivered 3682 production hours for users over 6 cycles
- 100% predictability
- Operated at 85 MW
- Completed 50 cycles with cold source

SNS

- Delivered 4424 production hours for users at 94.1% availability against planned hours
- Operated at ~1.0 MW and 60 Hz
- World record 1.4 MW for pulsed linac
- Developed plan to extend target life-time



Science program

- Supported 893 unique users at SNS and 453 unique users at HFIR
- Over 900 proposals received during last proposal call setting a new facility record
- HFIR is also an exceptional resource for materials irradiation and neutron activation analysis and continuing mission in isotope production

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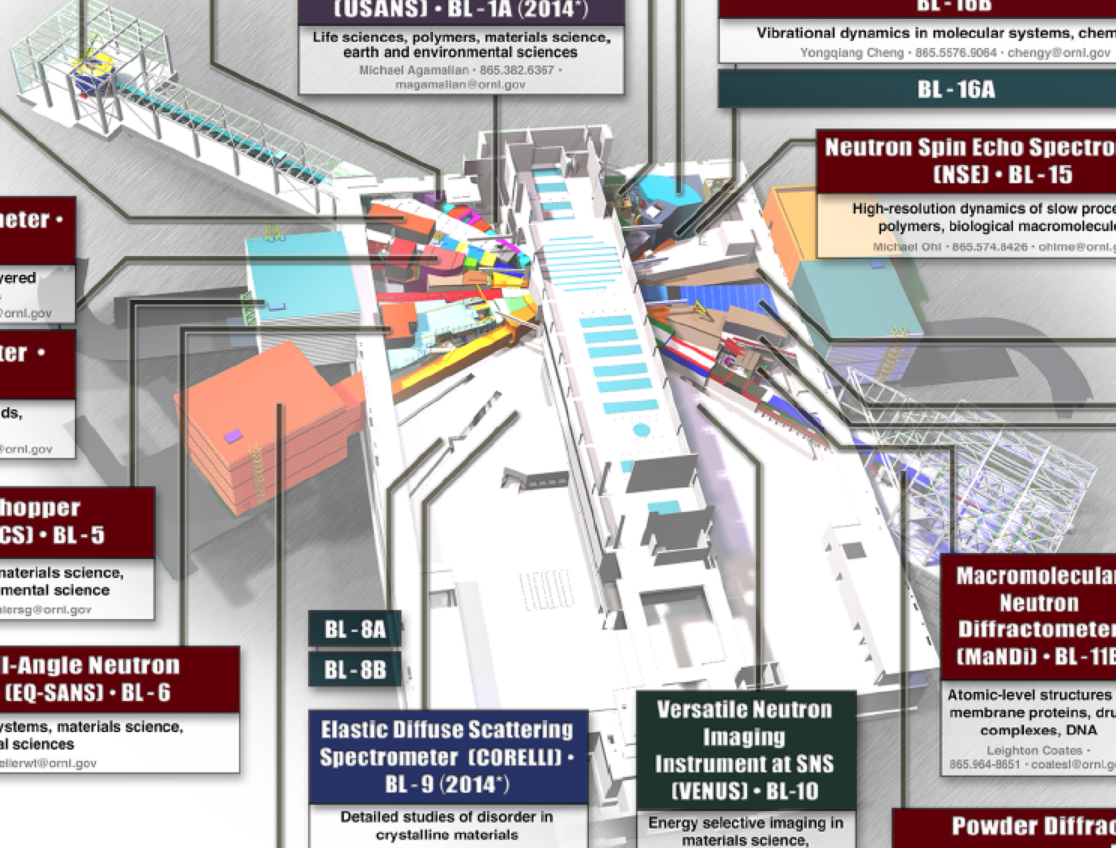
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

World's most intense pulsed, accelerator-based neutron source

NEUTRONS.ORNL.GOV



Backscattering Spectrometer (BASIS) • BL-2
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Eugene Mamontov • 865.574-5109 • mamontove@ornl.gov

Nanoscale-Ordered Materials Diffractometer (NOMAD) • BL-1B
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuefeind • 865.241.1635 • neuefeindjc@ornl.gov

Wide Angular-Range Chopper Spectrometer (ARCS) • BL-18
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Doug Abernathy • 865.617.5624 • abernathydl@ornl.gov

Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) • BL-17
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Matthew Stone • 865.202.6898 • stonemb@ornl.gov

Ultra-Small-Angle Neutron Scattering Instrument (USANS) • BL-1A (2014*)
Life sciences, polymers, materials science, earth and environmental sciences
Michael Agamalian • 865.382.6367 • magamalian@ornl.gov

Vibrational Spectrometer (VISION) • BL-16B
Vibrational dynamics in molecular systems, chemistry
Yongqiang Cheng • 865.5576.9064 • chengy@ornl.gov

BL-16A

Spallation Neutrons and Pressure Diffractometer (SNAP) • BL-3
Materials science, geology, earth and environmental sciences
Chris Tulk • 865.574.5764 • tulkca@ornl.gov

Neutron Spin Echo Spectrometer (NSE) • BL-15
High-resolution dynamics of slow processes, polymers, biological macromolecules
Michael Ohl • 865.574.8426 • ohlme@ornl.gov

Hybrid Spectrometer (HYSPEC) • BL-14B
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Barry Winn • 865.805.6819 • winnbl@ornl.gov

BL-14A

Magnetism Reflectometer • BL-4A
Chemistry, magnetism of layered systems and interfaces
Valeria Lauter • 865.387.5389 • lauterv@ornl.gov

Liquids Reflectometer • BL-4B
Interfaces in complex fluids, polymers, chemistry
John Ankner • 865.377.4523 • anknerjf@ornl.gov

Fundamental Neutron Physics Beam Line • BL-13
Fundamental properties of neutrons
Geoffrey Greene • 865.576.0023 • greenegl@ornl.gov

Cold Neutron Chopper Spectrometer (CNCS) • BL-5
Condensed matter physics, materials science, chemistry, biology, environmental science
Georg Ehlers • 865.206.0824 • ehlersg@ornl.gov

Macromolecular Neutron Diffractometer (MaNDi) • BL-11B
Atomic-level structures of membrane proteins, drug complexes, DNA
Leighton Coates • 865.964-8651 • coatesl@ornl.gov

Single-Crystal Diffractometer (TOPAZ) • BL-12
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
Christina Hoffmann • 865.576.5127 • choffmann@ornl.gov

BL-8A

BL-8B

Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) • BL-6
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
William Heller • 865.241.0093 • hellerwt@ornl.gov

Elastic Diffuse Scattering Spectrometer (CORELLI) • BL-9 (2014*)
Detailed studies of disorder in crystalline materials
Feng Ye • 865.576.0931 • yef1@ornl.gov

Versatile Neutron Imaging Instrument at SNS (VENUS) • BL-10
Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology
Hassina Bilheux • 865.384.9630 • bilheuxhn@ornl.gov

Powder Diffractometer (POWGEN) • BL-11A
Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures
Ashfia Huq • 630.986.7321 • huqa@ornl.gov

Engineering Materials Diffractometer (VULCAN) • BL-7
Mechanical behaviors, materials science, materials processing
Ke An • 865.919.5226 • kean@ornl.gov

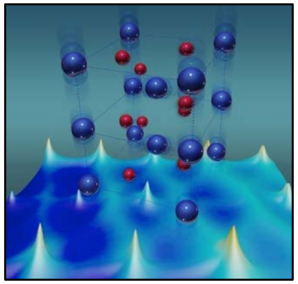
*Scheduled commissioning date

LEGEND
- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

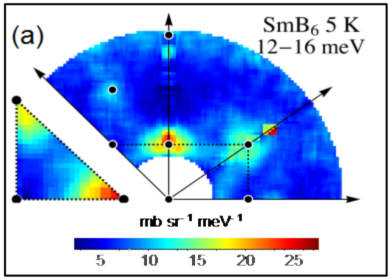
14-G00875/gim

The Spallation Neutron Source is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

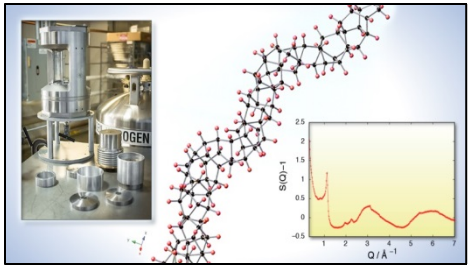
The HFIR and SNS user program is delivering high impact science



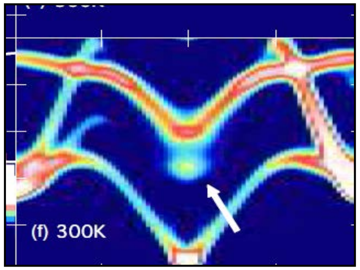
Budai *et al.*
Nature (2014)



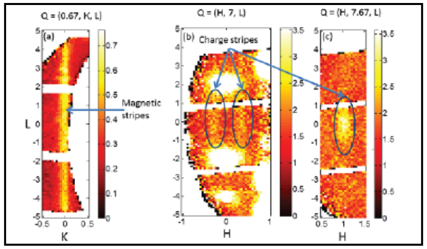
Fuhrman *et al.*
Phys. Rev. Letters (2015)



Fitzgibbons *et al.*
Nature Materials (2015)

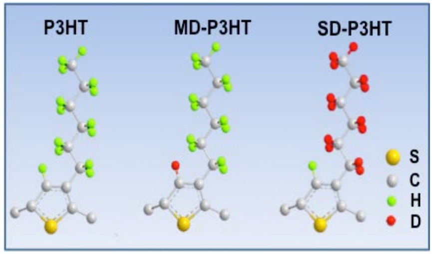


Li *et al.*
Phys. Rev. Letters (2014)

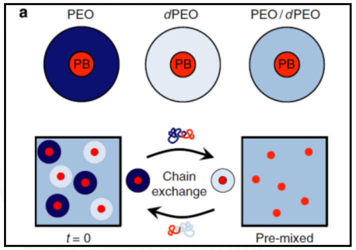


Anissimova *et al.*
Nature Comm. (2014)

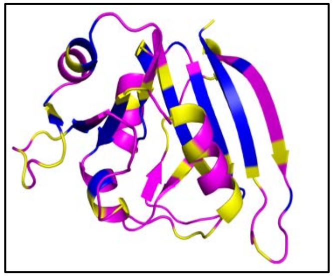
Santodonato *et al.*
Nature Comm. (2015)



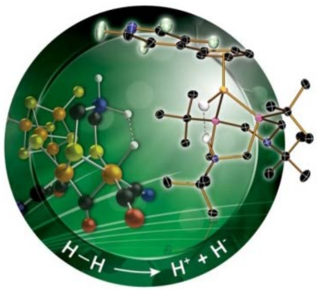
Shao *et al.*
Nature Comm. (2014)



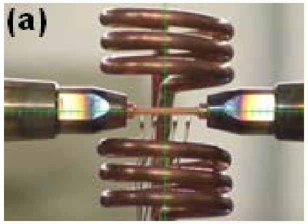
Kelley *et al.*
***Nature Comm.* (2014)**



Wan *et al.*
Proc. Nat. Acad of Sci. (2014)



Liu *et al.*
Angew. Chem. Int. Ed. (2014)



Stoica *et al.*
Nature Comm. (2014)

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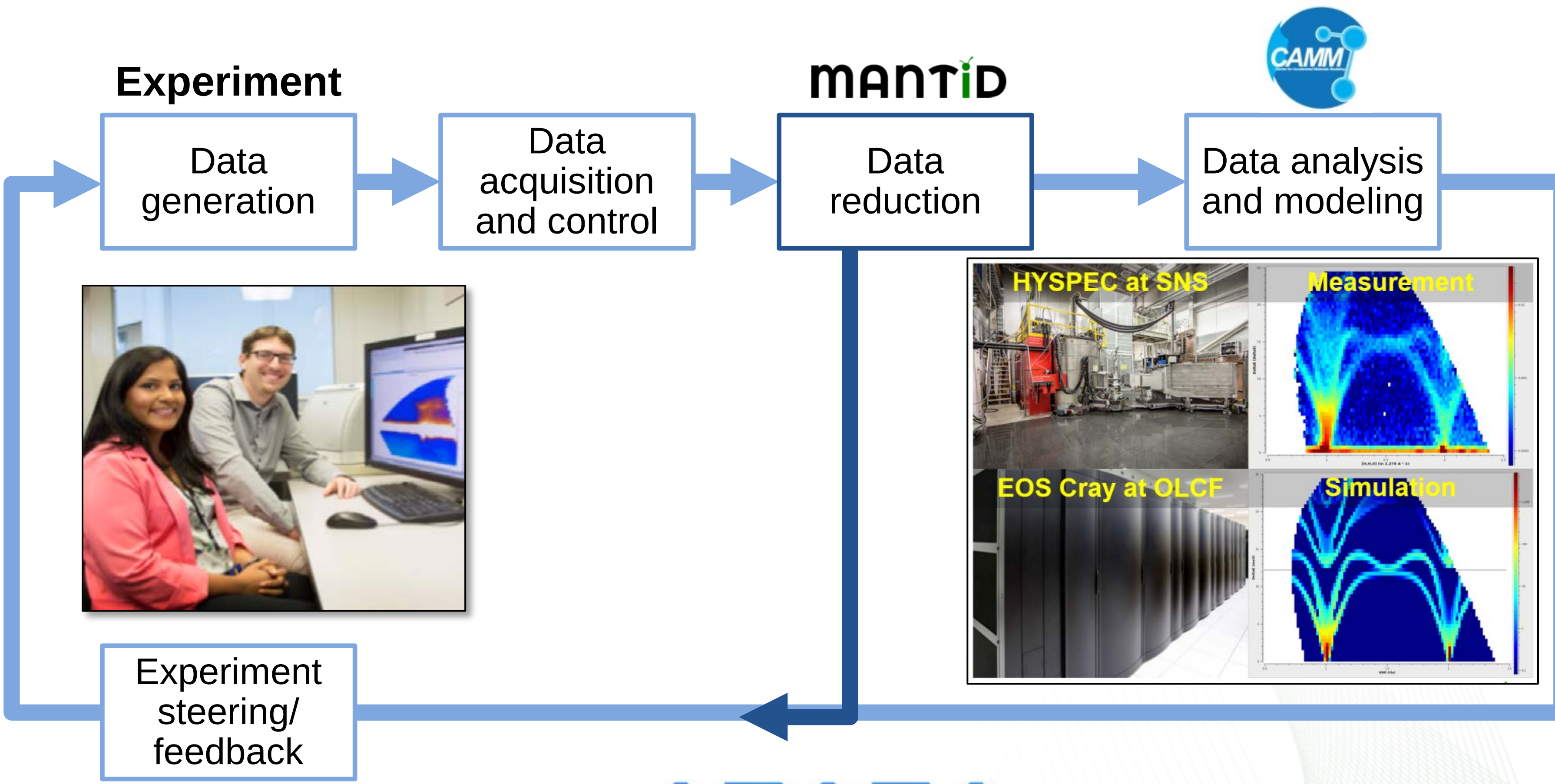
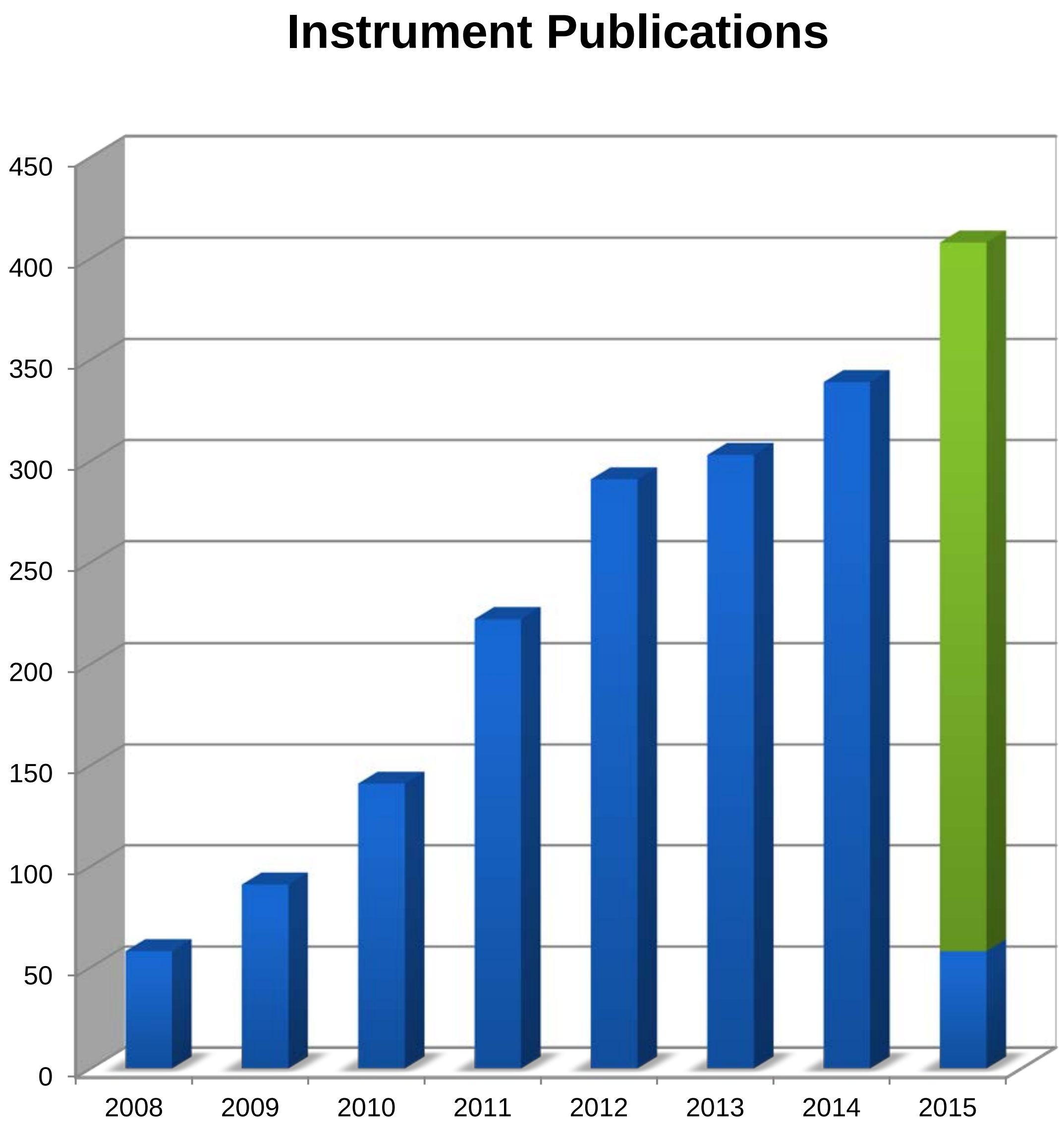
Moving data analysis, modeling and simulation closer to the experiment

Research Details: Ferroelectric instabilities in $SrTiO_3$ (HYSPEC at SNS) using live data streaming. Full scale AIMD simulations (Cray XC30 EOS cluster at OLCF with 11,000 cores) on experiment timescale allowing real time decisions.

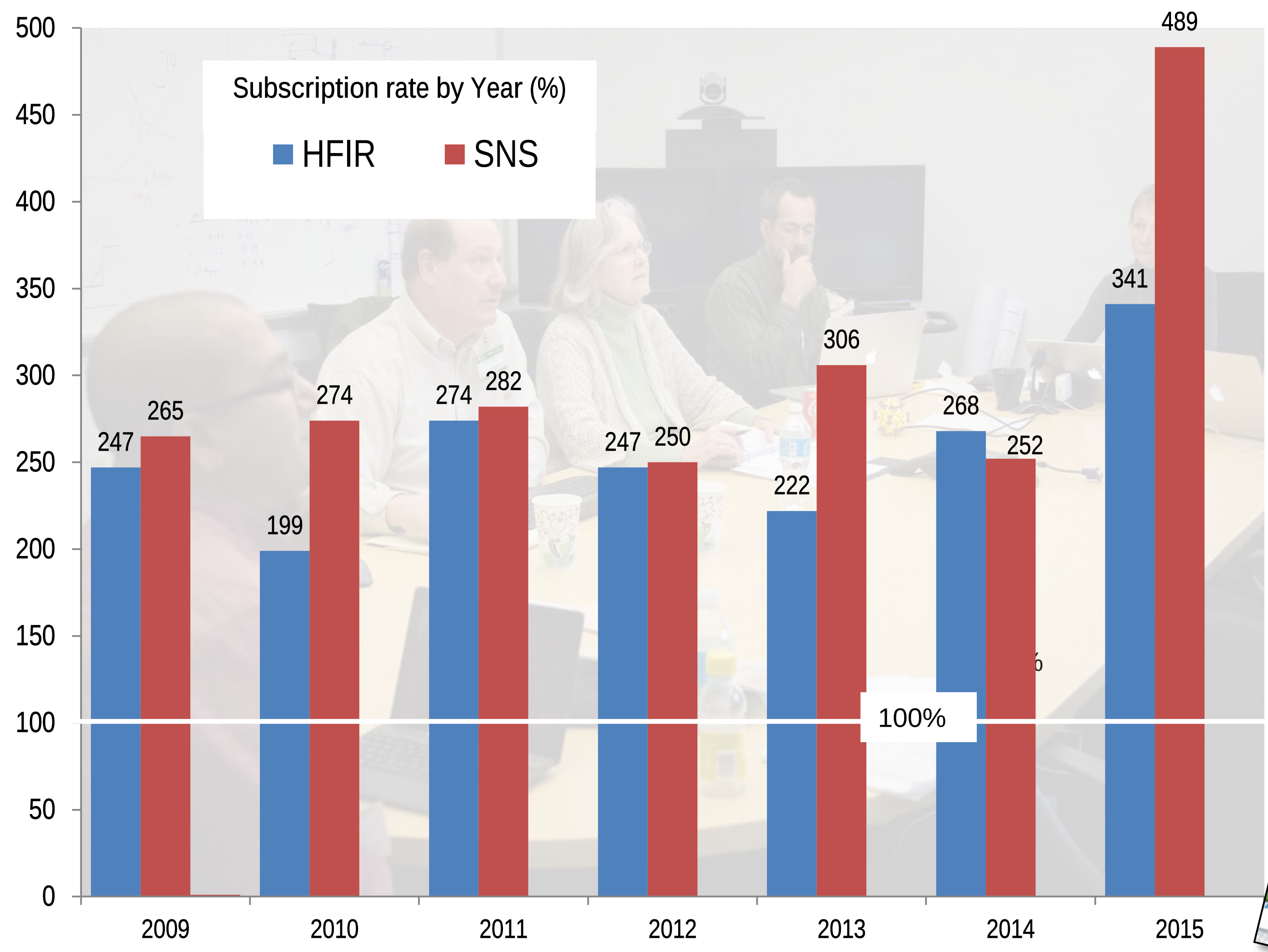


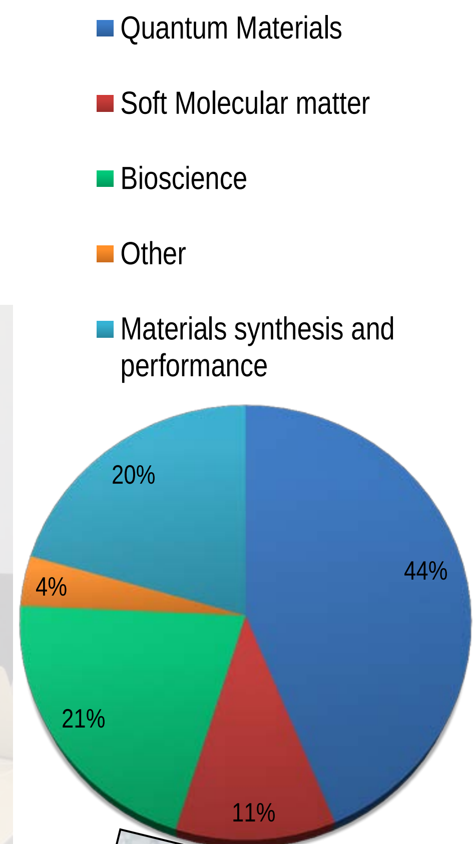
Accelerating Data Acquisition, Reduction, and Analysis

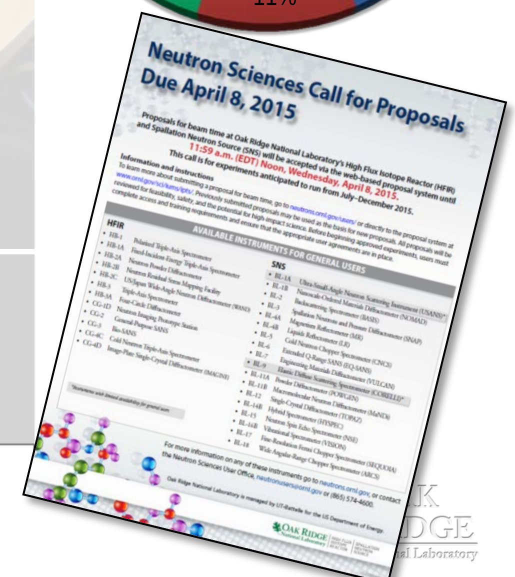
Scientific productivity is on a strong upward trend



All instruments are oversubscribed






Neutron Sciences Call for Proposals
Due April 8, 2015

Engaging the scientific community to identify emerging science challenges that neutrons can address

Quantum Materials

Quantum Condensed Matter
Lawrence Berkeley National Laboratory
December 2013
Bob Birgeneau

Biosciences

Structural Biology, Bio-materials, and Bioengineering
UC San Diego
January 2014
Susan Taylor

Soft Molecular Matter

Soft Matter
Santa Barbara
May 2014
Fyl Pincus
and Matt Tirrell

Materials Synthesis and Performance

Energy Materials
Chicago
August 2014
George Crabtree
and John Parise

Frontiers in Data Modeling and Simulation Argonne Nat. Lab. March 30-31, 2015
Peter Littlewood

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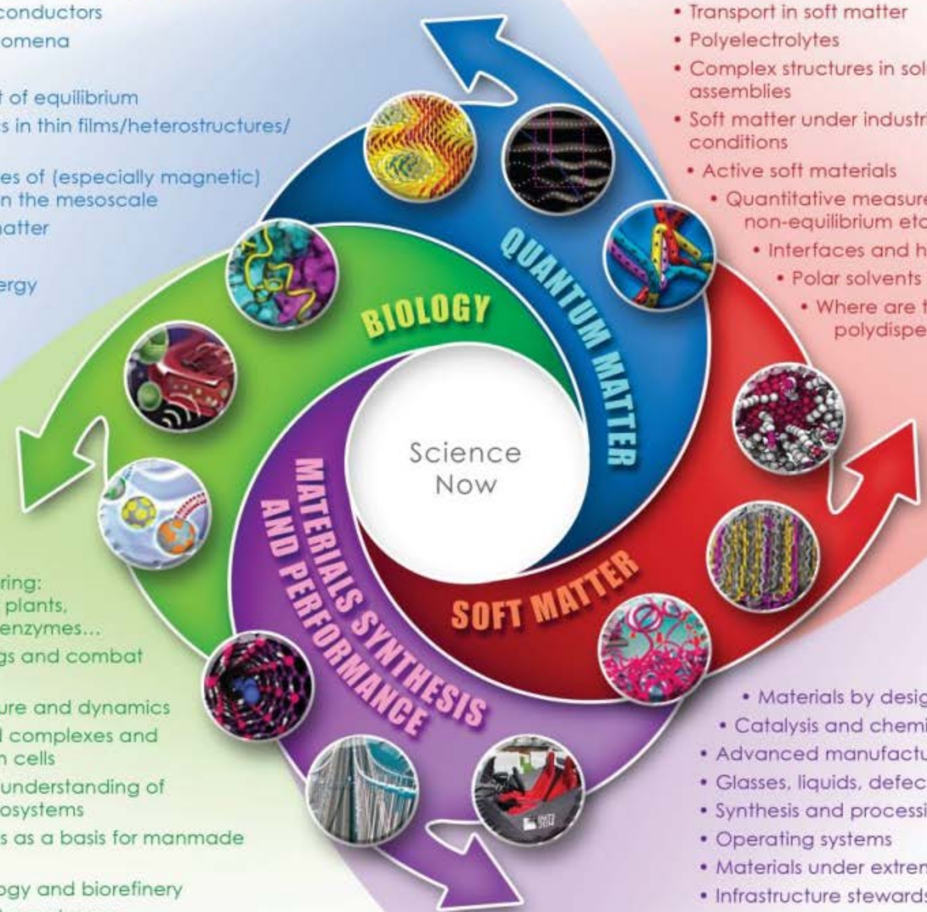
Next Generation Science

- Exotic ground states in quantum magnets
- Unconventional Superconductors
- Quantum Critical Phenomena
- Itinerant Magnets
- Quantum materials out of equilibrium
- Structure and dynamics in thin films/heterostructures/ nanomaterials
- Spatially resolved probes of (especially magnetic) structure of materials on the mesoscale
- Topological states of matter
- Hydrogen in materials
- Strongly correlated energy materials
- Determining the structure of partially ordered materials including defect structures

- Response of mechanical deformation
- Soft/hard matter composites
- Transport in soft matter
- Polyelectrolytes
- Complex structures in solution/Heirarchical assemblies
- Soft matter under industrial processing conditions
- Active soft materials
- Quantitative measurements : curvatures, non-equilibrium etc.
- Interfaces and hybrid systems
- Polar solvents other than water
- Where are the effects of polydispersity



- Bioengineering: redesign of plants, organisms, enzymes…
- Design drugs and combat resistance
- Unify structure and dynamics
- Understand complexes and processes in cells
- Integrated understanding of complex biosystems
- Biomaterials as a basis for manmade systems
- Biotechnology and biorefinery
- Understand membranes
- Disorder and flexibility in signaling, communications, regulation
- Kinetics within multi-protein systems

- Materials by design
- Catalysis and chemical reactions
- Advanced manufacturing
- Glasses, liquids, defects and disorder
- Synthesis and processing
- Operating systems
- Materials under extreme conditions
- Infrastructure stewardship
- Future energy and transport
- Porous materials
- Gas absorption
- Pharmaceuticals

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Concepts for next-generation instruments and sources
-being developed and demonstrated through LDRD

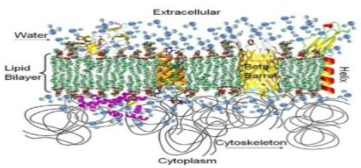
Higher flux on sample: Compact moderators; beam optics

Improved detectors: High data rates and resolutions

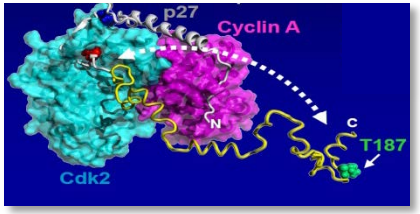
Polarized beams: Spin nutators and manipulators

Computation: Hierarchy and mesoscale; slow dynamics

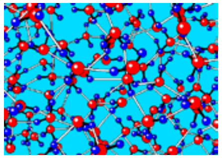
STS can deliver transformative capabilities for complex systems



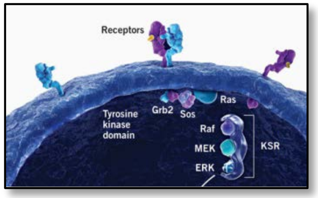
Biological membranes and associated complexes



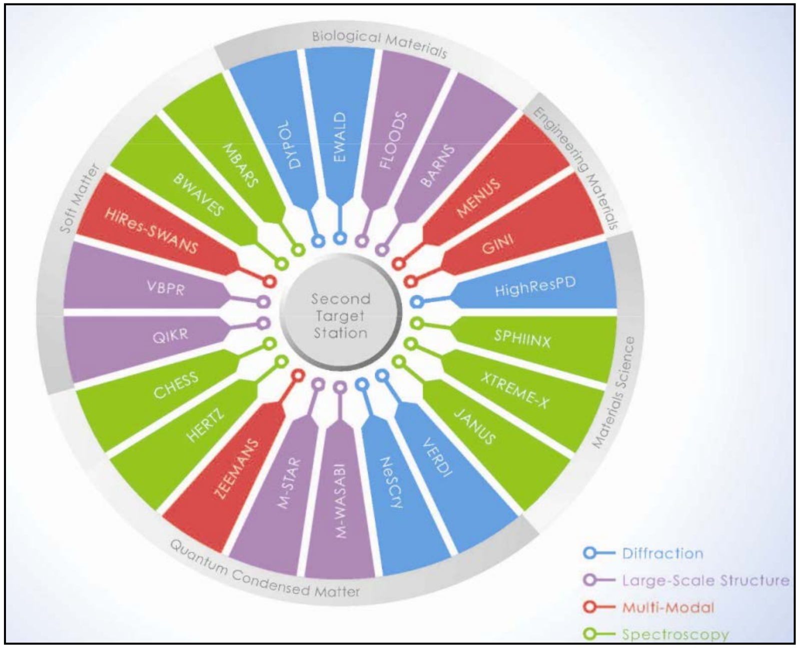
Disorder and flexibility



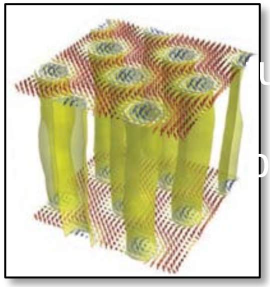
Reactions, catalysis, and kinetics



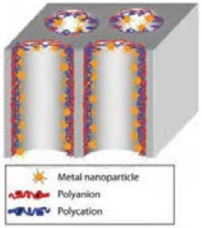
Dynamic functional assemblies



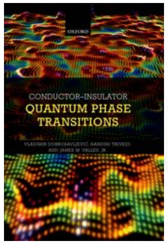
Novel manufacturing and processing



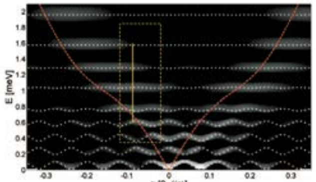
Topological materials and excitations



Hierarchical materials



Extreme conditions and new phases of matter



Artificial crystals and heterostructures

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Complementarity across 3 ORNL neutron sources provides opportunity for instrument optimization

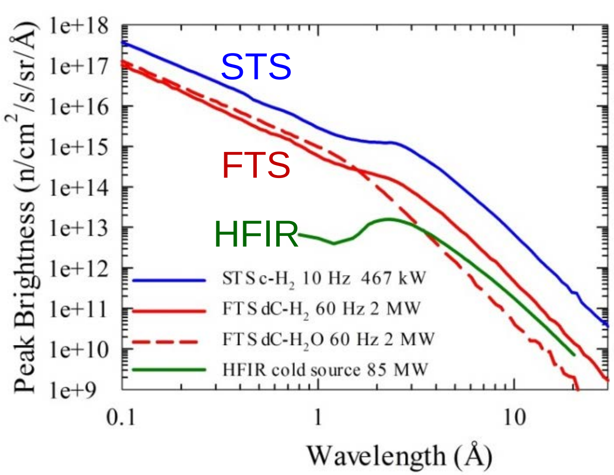
STS: Optimized for cold neutrons with high peak brightness

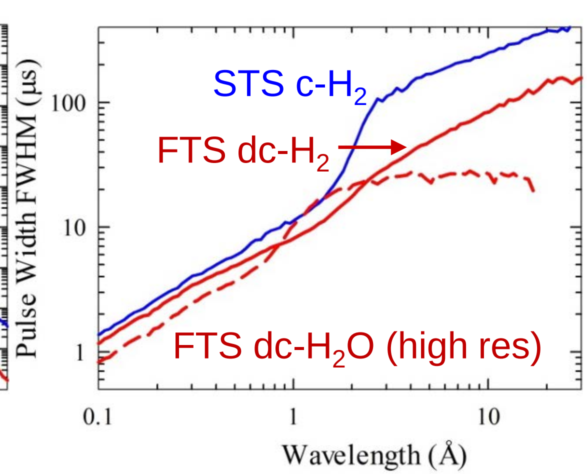
(Coupled moderators, 10 Hz)

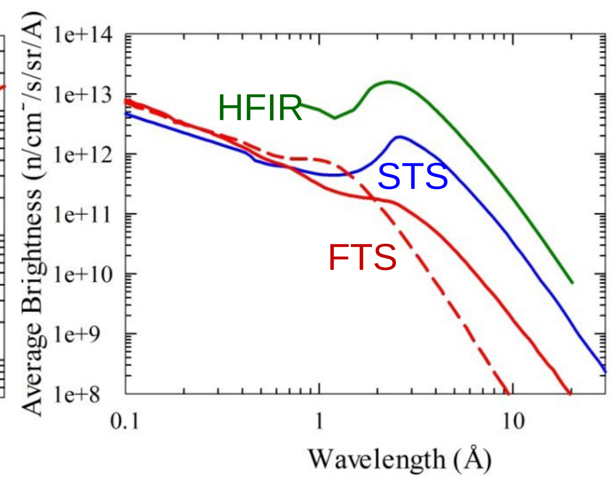
FTS: Optimized for high-wavelength resolution across neutron spectrum

(Decoupled moderators, 60 Hz)

HFIR: Optimized for cold and thermal neutrons with high time-averaged brightness







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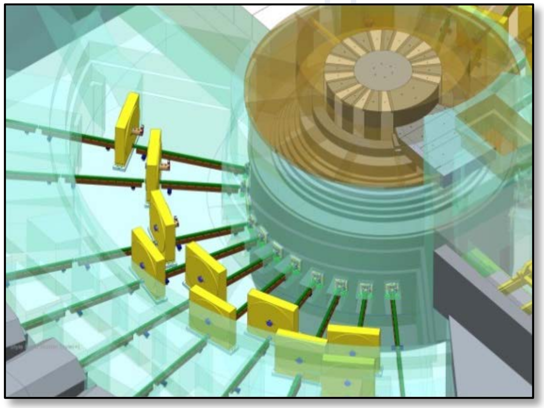
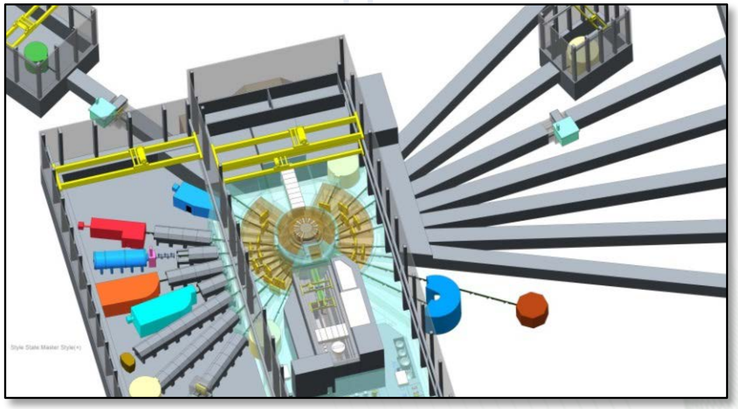
TDR activities, FY 2014

Core team of engaged individuals

Establish initial design concepts	Define Work Breakdown Structure to level 3	Engage A/E for site layout and definition of conventional facilities
• Plan for instrument suite • 3 moderators (FY13 LDRD) • Compact tungsten target • Proton beamline lattice to STS	• Major subsystems (e.g., individual instruments, accelerator RF systems) • Top-down cost estimates	• ORNL estimators will generate initial cost estimate





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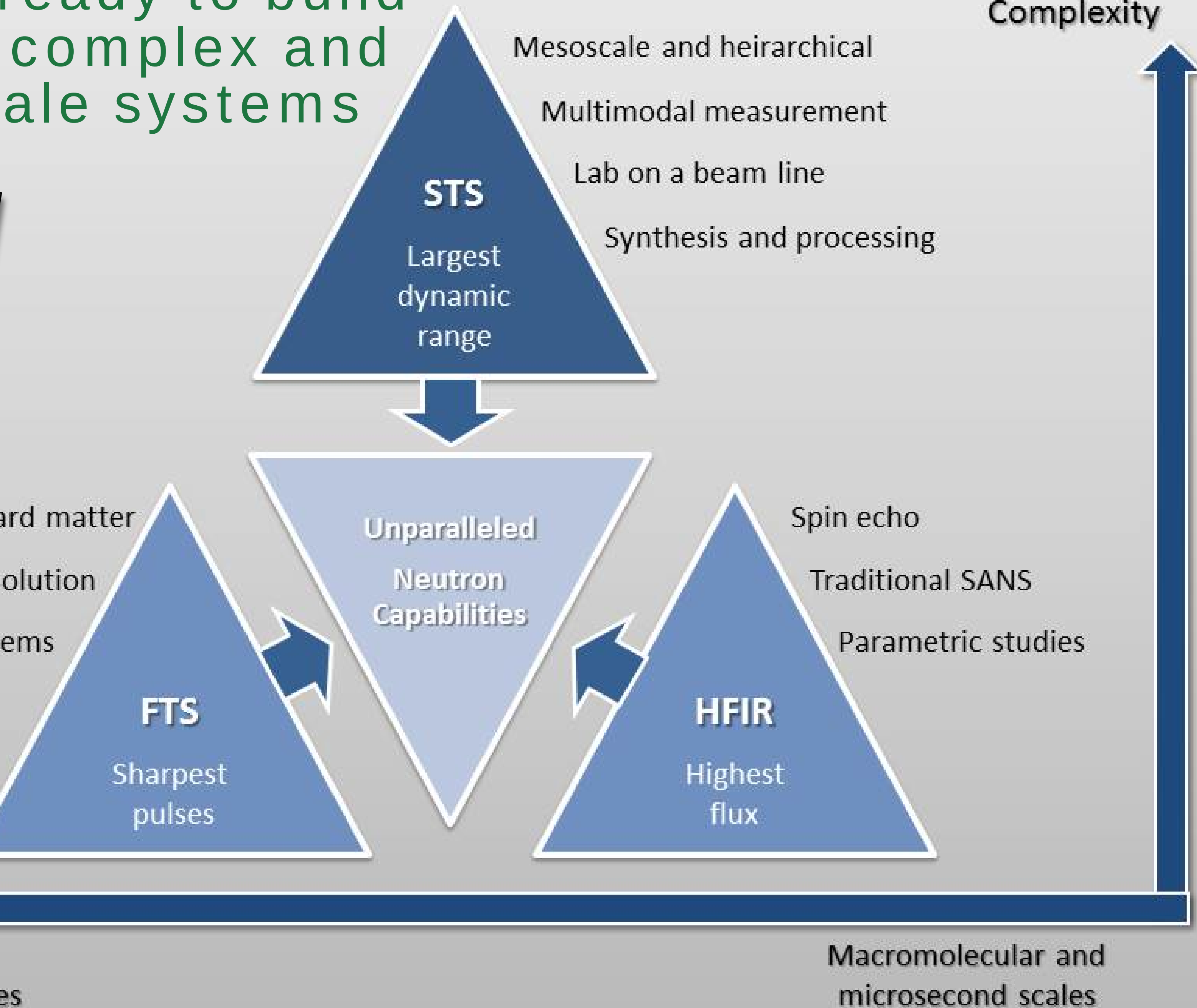
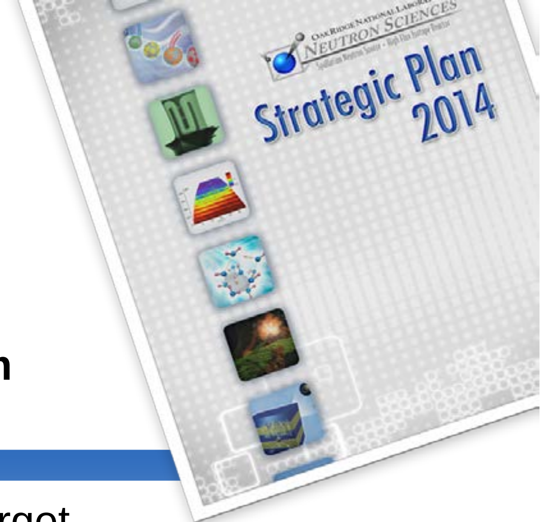
We are ready to build STS for complex and mesoscale systems



Best neutron capabilities for researchers to address the most important emerging challenges



Science priorities

Defined through broad community engagement

- Soft molecular matter
- Quantum materials
- Materials synthesis and performance
- Biosciences

Near-term focus

Maximize scientific impact at SNS and HFIR

- Facility improvement
- New technologies and methods for next generation science
- Integration with computational methods and other exp. techniques

Long-term plan

Second target station at SNS to double neutron science capacity and expand capabilities by 2-3 orders of magnitude, new capabilities for complexity

- Optimize science across complementary sources
- Positioning to address the emerging grand challenges of our sponsors and research community

Summary

- HFIR and SNS are producing high impact science
- Scientific productivity is on a strong upward trend
- The user community is being engaged to look to the future and define the emerging grand challenges
- We are responding to those challenges by developing new concepts and technologies for next generation instruments and sources.
- Our short term focus is on maximizing the capabilities of the SNS and HFIR
- Our long term focus is on building a second target station at the SNS
- We aim to provide the best possible neutron capabilities for researchers to use to address the biggest and most important problems