Welcome to the

Review of Instrument Suite for Spectroscopy

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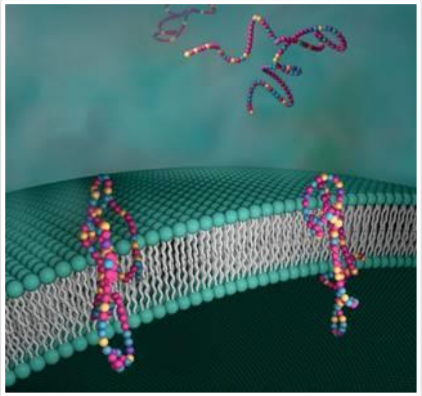
Sept. 17-18, 2020

Conference.sns.gov/event/242
PW: nsdbr20

Advance impact and application of neutron science

Vision

- SNS and HFIR are world-leading centers for neutron scattering science and innovation, providing unparalleled capabilities for discovery science and solving the most challenging research problems



Artificial proton channels through membranes
Jiang et al., *Nature* 2020

Strategy

- Enhance neutron scattering capabilities for users by delivering world-leading thermal and cold neutron sources
- Couple neutron scattering capabilities with other synthesis, characterization, and computational tools, enabling self-driven experiments
- Assess potential for extending HFIR's lifetime and enhancing its capabilities
- Deliver new instruments, sample environments, and data analytics

Science priorities

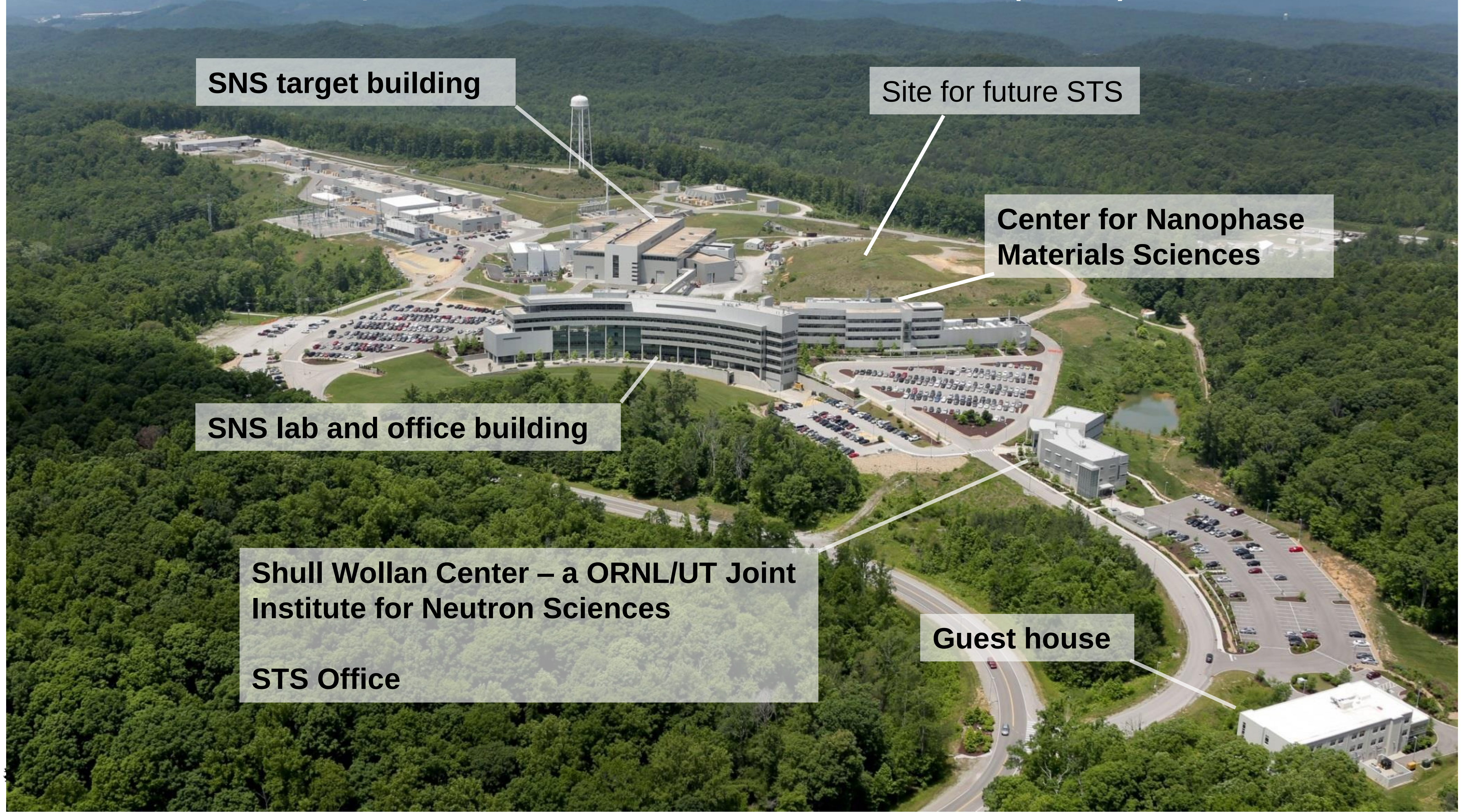
- Discover and characterize quantum effects that can be controlled in novel materials, underpinning transformational technologies
- Understand how hierarchical structures with desired materials properties can enable breakthroughs in novel materials
- Reveal how structure and dynamics of biological systems can be used in new applications in energy, biotechnology, and biosecurity

Recent achievements

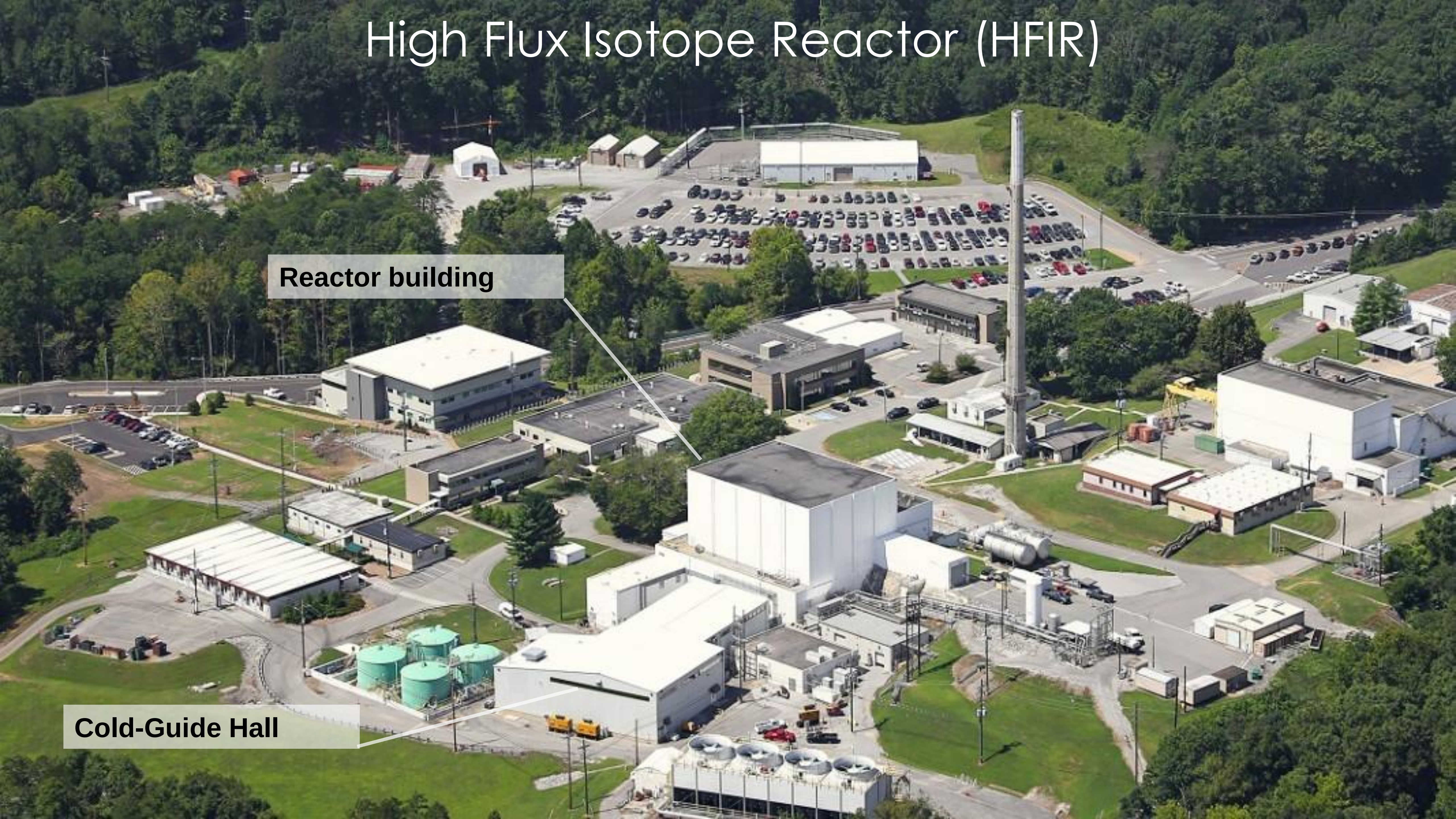
- SNS: Sustained operation (95% reliability) at 1.4 MW
- HFIR: Re-established safe and reliable operations
- Proton Power Upgrade (PPU): CD-3B approved; construction in progress
- Second Target Station (STS): Project leadership in place; pursuing CD-1
- Versatile Neutron Imaging Instrument (VENUS) under construction
- CY19: 677 publications

Aerial view of Oak Ridge National Laboratory

Spallation Neutron Source (SNS)



High Flux Isotope Reactor (HFIR)



HFIR and SNS are operating with exceptional reliability, but user program is constrained by COVID-19

- HFIR has completed 6 cycles as scheduled since its restart on Oct. 29, 2019
- SNS's FY 2020 neutron production availability exceeds >95%
- No on-site users since March 2020
  - Both SNS and HFIR restarted after their respective outages to initially perform only COVID-19 research
  - We have gradually restarted all instruments for activities beyond COVID-19 research
  - On-site presence is limited to less than half of Neutron Scattering Division personnel
  - 180 Remote Access Experiments performed, with 200 remote participants from 78 institutions

Neutron Sciences Directorate

Second Target Station Project

Comp. and Comp. Sci. Dir

- Research Reactors Division
- Research Accelerator Division
- Neutron Scattering Division
- Neutron Technologies Division
- Proton Power Upgrade Project
- Scientific and Program Services
- Comp. Sci. and Math. Division

Neutron Scattering Division:

- Diffraction
- Materials Engineering
- Large Scale Structures
- Spectroscopy
- Beamline Support
- Sample Environment

Comp. Sci. and Math. Division:

- Research Software Engineering

Diffraction

BL-1B	NOMAD
BL-9	CORELLI
BL-11A	POWGEN
BL-11B	MaNDi
BL-12	TOPAZ
HB-2A	POWDER
HB-2C	WAND[2]
HB-3A	DEMAND
CG-3D	IMAGINE

Materials Engineering

BL-3	SNAP
BL-7	VULCAN
BL-10	*VENUS*
HB-2B	HIDRA
CG-1D	IMAGING

Large Scale Structures

BL-1A	USANS
BL-4A	MagREF
BL-4B	LiqREF
BL-6	EQ-SANS
BL-15	NSE
CG-2	GP-SANS
CG-3	Bio-SANS

Spectroscopy

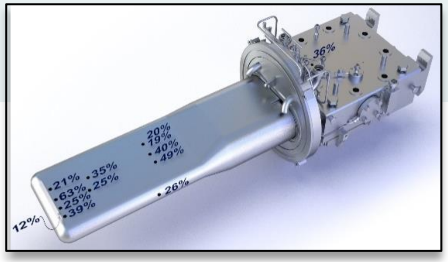
BL-2	BASIS
BL-5	CNCS
BL-14B	HYSPEC
BL-16B	VISION
BL-17	SEQUOIA
BL-18	ARCS
HB-1	PTAX
HB-1A	FIE-TAX
HB-3	TAX
CG-4C	CTAX

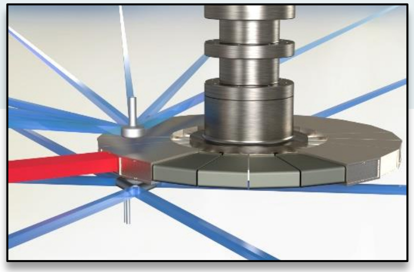
Science Initiatives:

Biological Materials & Systems
Chemistry, Catalysis, and Interfaces
High Performance Computing, Modeling, and Data Analytics
High Pressure Science
Materials and Engineering
Quantum Materials
Soft Matter and Polymers

Context: ORNL's Three-Source Strategy

Current		Future
HFIR	SNS FTS	SNS STS
• High time-integrated flux for both cold and thermal neutrons • Polarized neutrons • Focusing monochromators	• High repetition rate • High resolution • Focused bandwidth • Thermal and epithermal neutrons	• High peak brightness of cold neutrons • Large bandwidth • Small beams
• Focused information in particular volumes of reciprocal space and energy • Parametric studies • Beamlines designed for flexible access and complex sample environments • Imaging	• High-resolution crystallography • Fast and high-energy dynamics • ToF Imaging	• Time-resolved studies • Hierarchical architectures • Kinetic processes in situ and operando • Studies at earliest stages of materials discovery



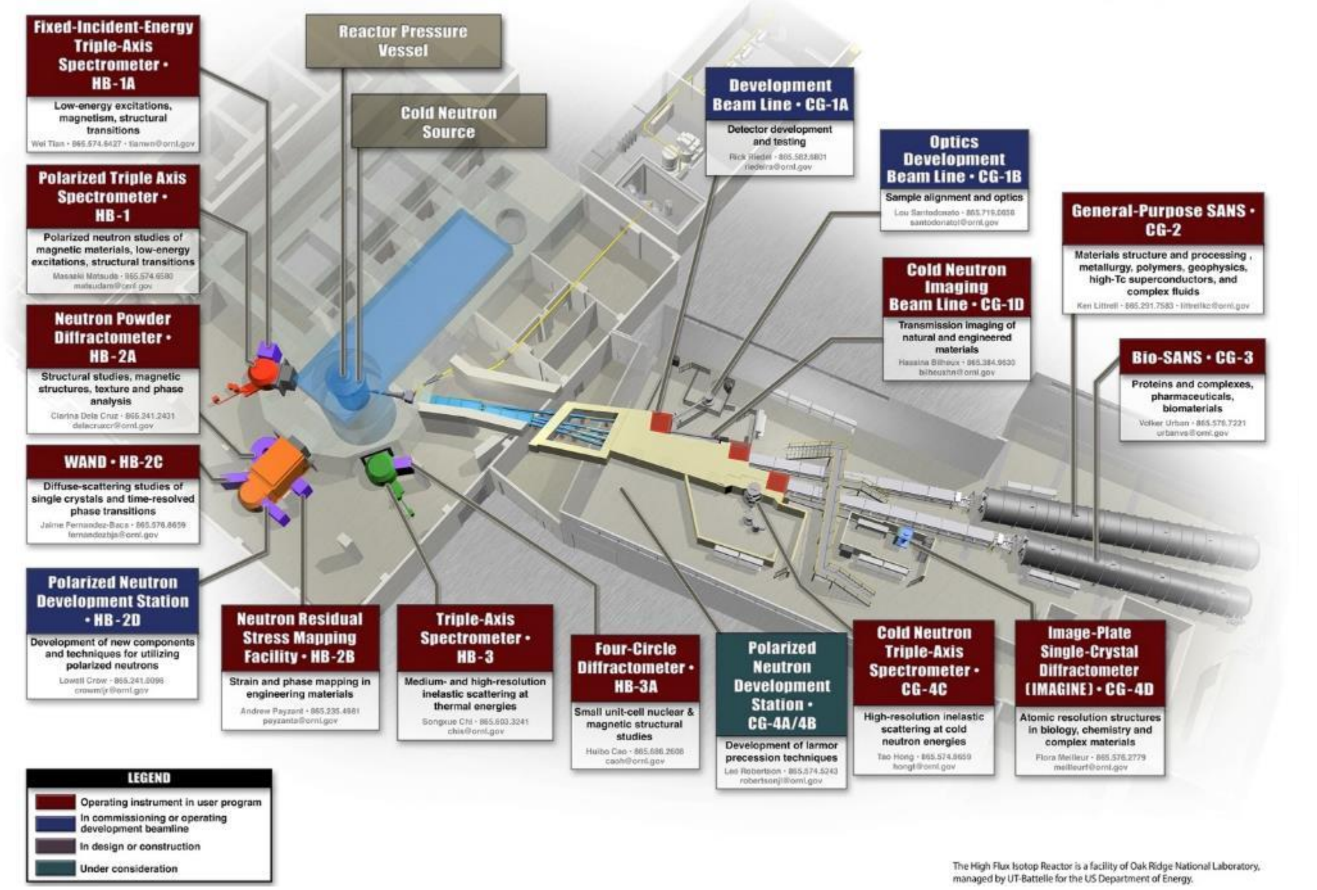


HFIR's Beryllium reflector replacement (2024): a challenge and an opportunity

- Required actions:
  - Completely remove instruments from Beam Room before outage; reinstall after outage
  - Completely remove instruments, guides, and shielding from Guide Hall during outage; reinstall after outage
  - Actual reactor shut-down of ~1 year; each neutron scattering instruments will be shut down for 18-24 months

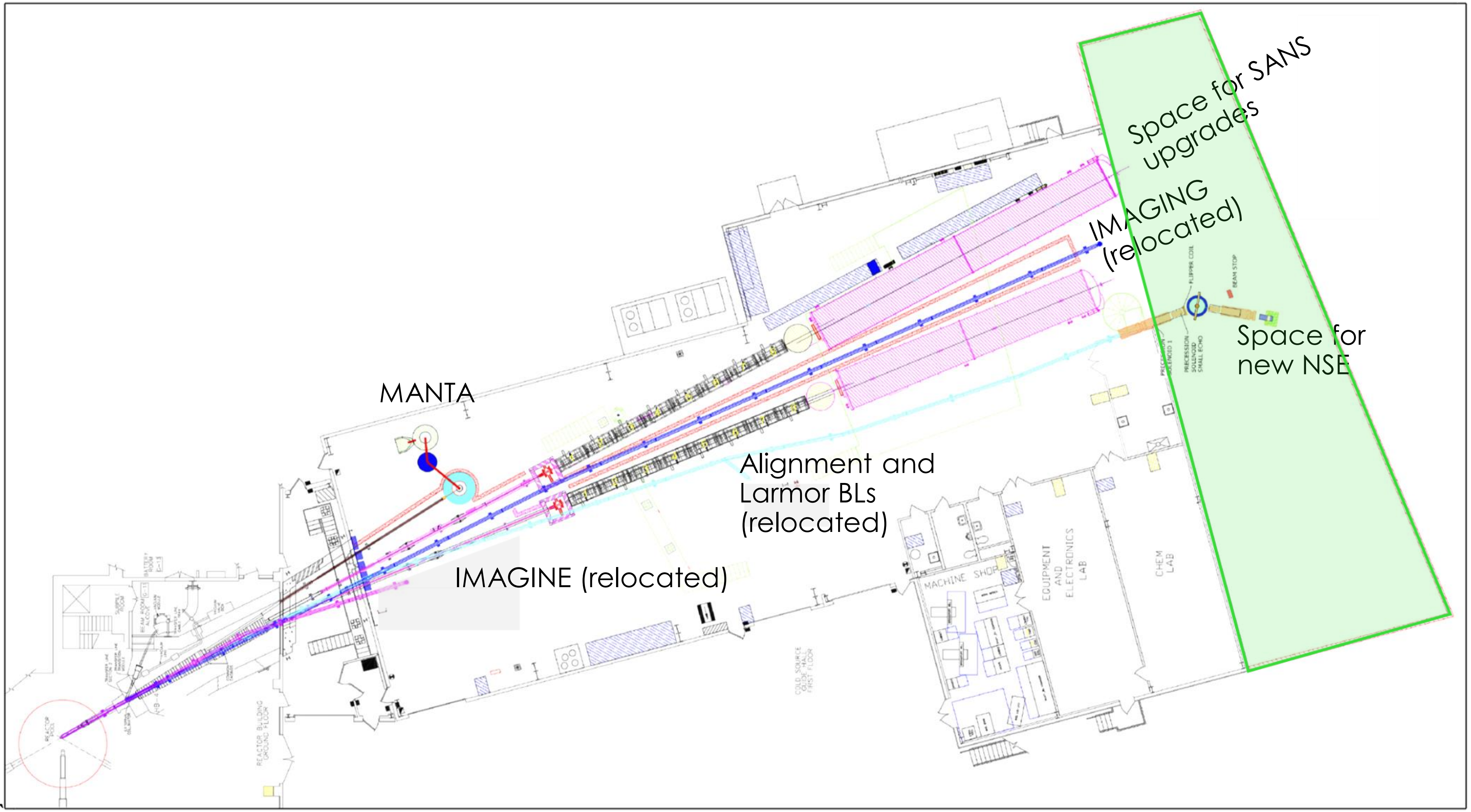
The Be-reflector replacement provides an opportunity to expand the current Cold-Source Guide Hall

- Current space is insufficient to maintain and improve capabilities:
  - MANTA (upgrade from CTAX)
    - Requires new location (displacing Imaging)
  - Maintain existing imaging capabilities
  - Create opportunities for NSE and future SANS improvements



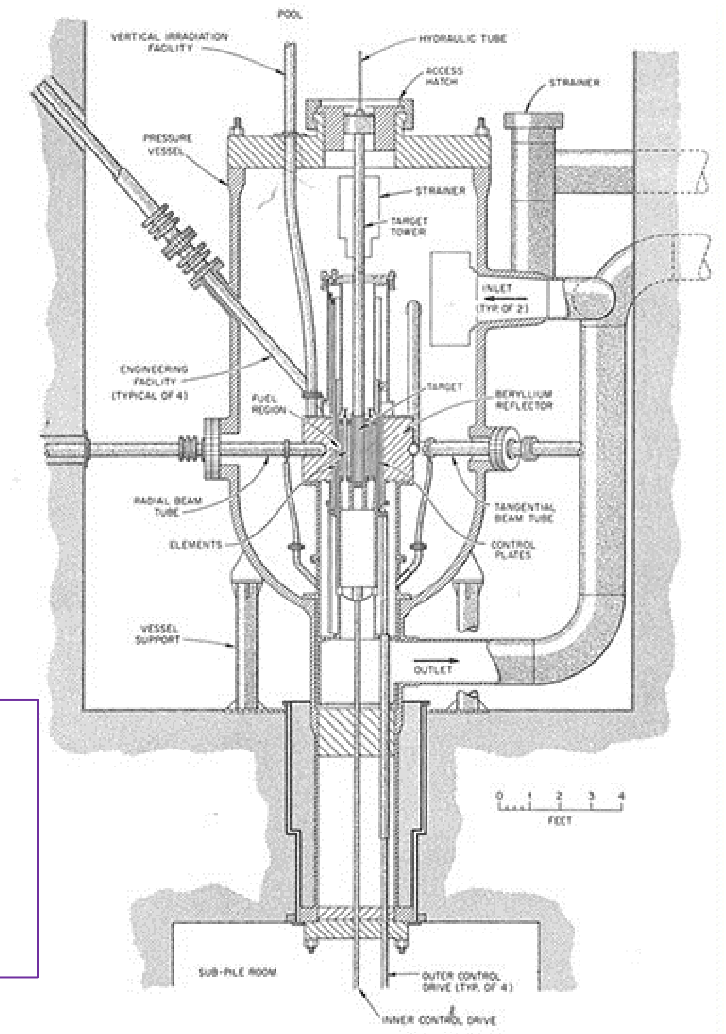
Discussed with user community at workshop before the American Conference on Neutron Scattering in June 2018

The planned Guide Hall Expansion will add 4,200 sq. ft



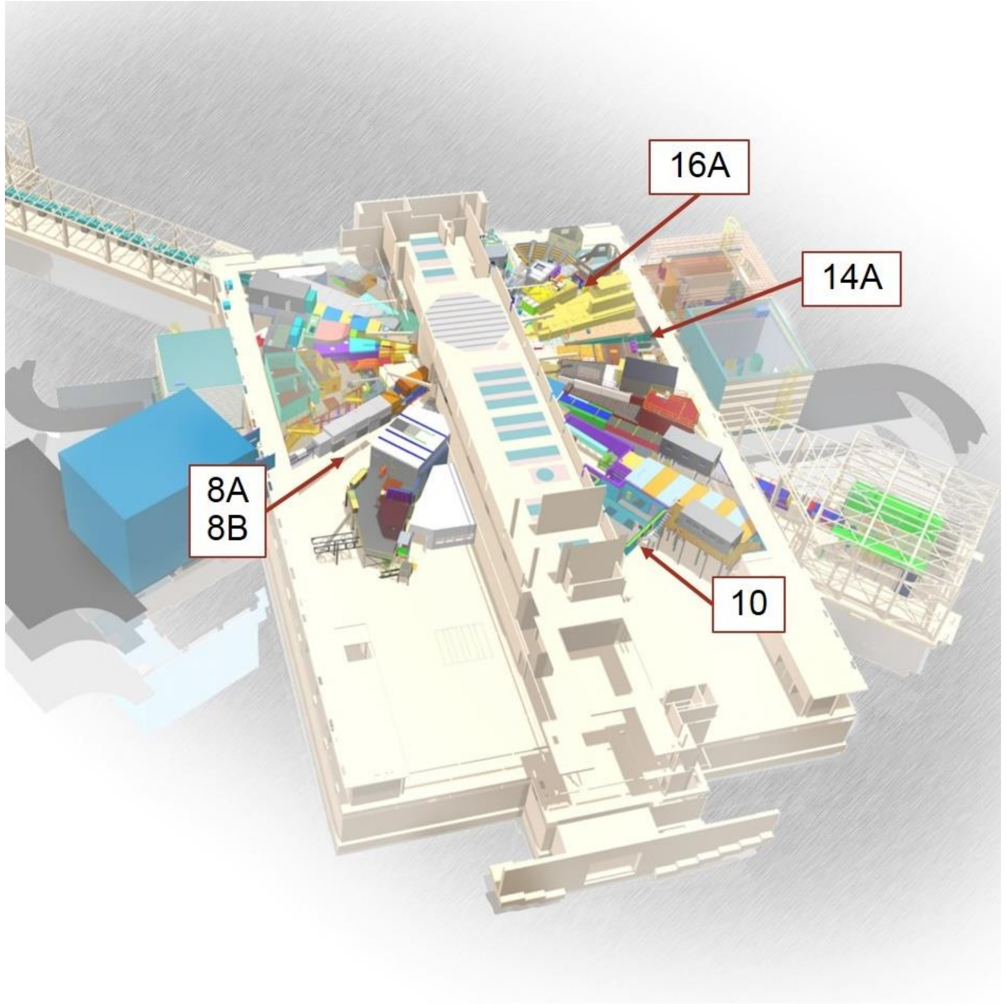
Long-term vision: A future pressure vessel replacement will provide an opportunity for significant enhancements

- **New pressure vessel**:
  - Operating at 100 MW (instead of 85 MW)
  - Extending life of HFIR by 50 years
- **D_2O reflector:**
  - Significant performance gain
- **Second guide hall at HB-2**:
  - ~10 instruments at much lower background
- **Upgraded cold source:**
  - ~50% higher brightness for neutron at $\lambda > 2$ Å



Replacing the pressure vessel is recommended in the BESAC Subcommittee Report (Robert Birgeneau, David Robertson) "The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility" (July 30 BESAC Meeting)

SNS: Currently unoccupied beam lines provide opportunities for new instruments



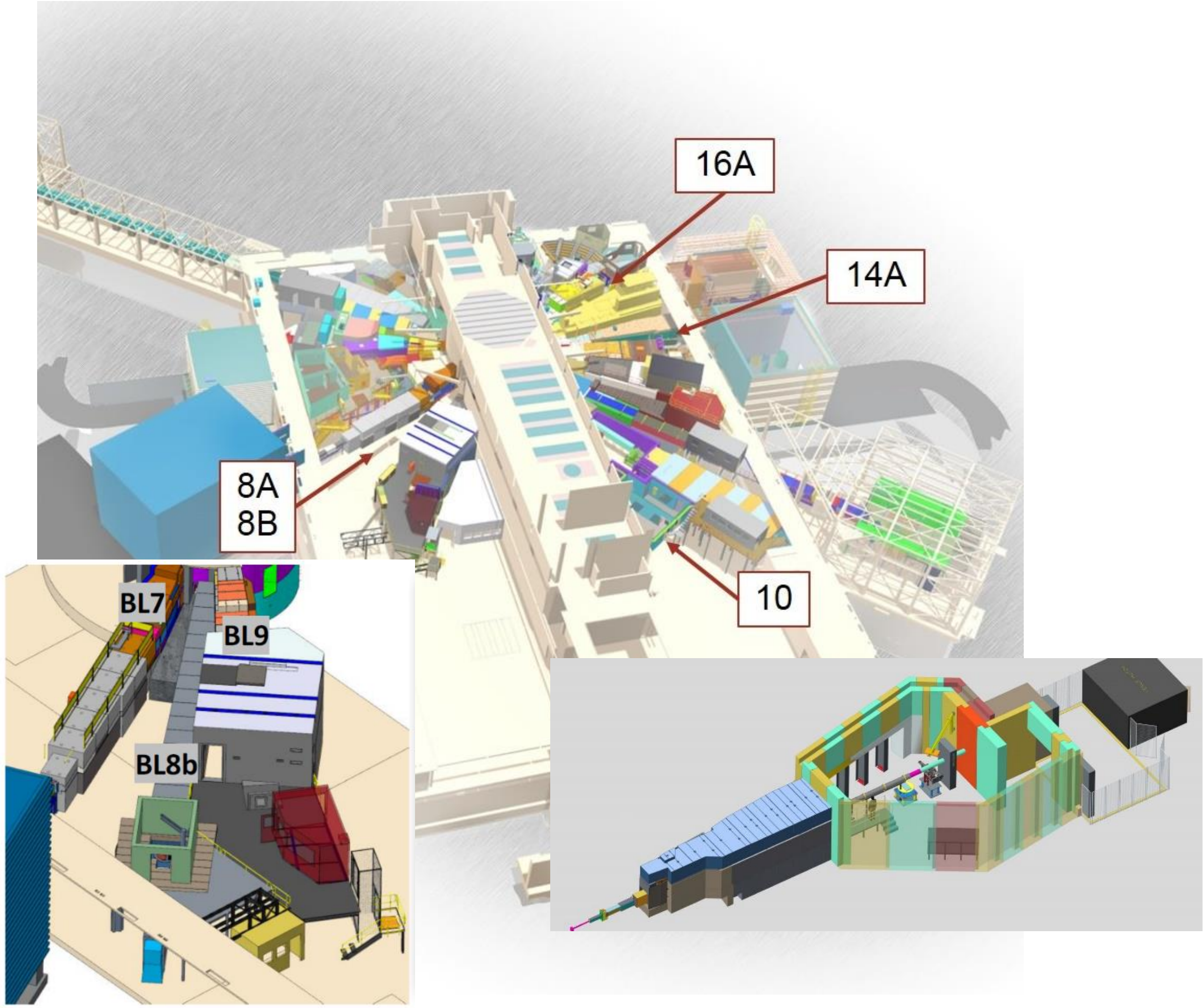
HIGGS	Inverse geometry spectrometer	BL-8A dc-p H_2O
MICRON	Compact, texture, special purpose diffractometer	
DISCOVER	Medium resolution/flux diffractometer	BL-8B dc-p H_2O
VENUS	Time-of-flight neutron imaging station	BL-10 dc-p para-H_2
INVENT	Concept development station	BL-14A c para-H_2
SANS/GI-SANS	SANS and/or GI-SANS	
BeFAST	Beryllium filter spectrometer	BL-16A dc-p H_2O
HiResPD	High Resolution Powder Diffractometer	Needs dc-p para-H_2 100 m flight path

dc-p: decoupled, poisoned
c: coupled
H_2O: thermal neutrons
para-H_2: cold neutrons

Discussed with user community at workshop before the American Conference on Neutron Scattering in June 2018

OAK RIDGE National Laboratory

Currently unoccupied beam lines at SNS provide opportunities for new instruments



VENUS (BL-10)

Under construction (1/1/2019 – 3/31/2023).

- Time-of-flight imaging
- Bragg-edge imaging, neutron resonance imaging, stroboscopic imaging

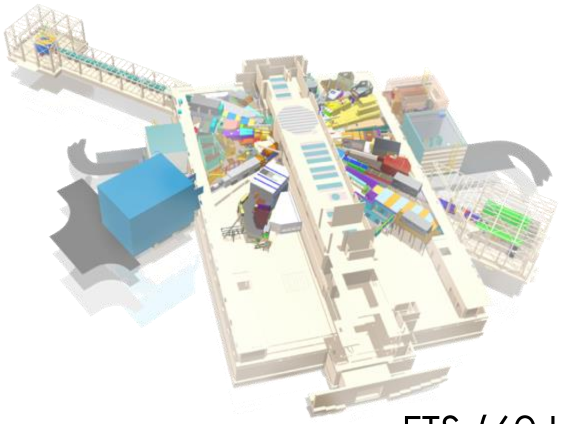
DISCOVER (BL-8B)

Planned.

- Rapid acquisition, medium-resolution, low background diffractometer
- Materials discovery, evolution, response.

SNS upgrade plans: Proton Power Upgrade (PPU) and STS

Today



FTS (60 Hz)

- 24 instrument positions
- 19 instruments built
- 2 instruments under construction or planned

1.4 MW

Accelerator today

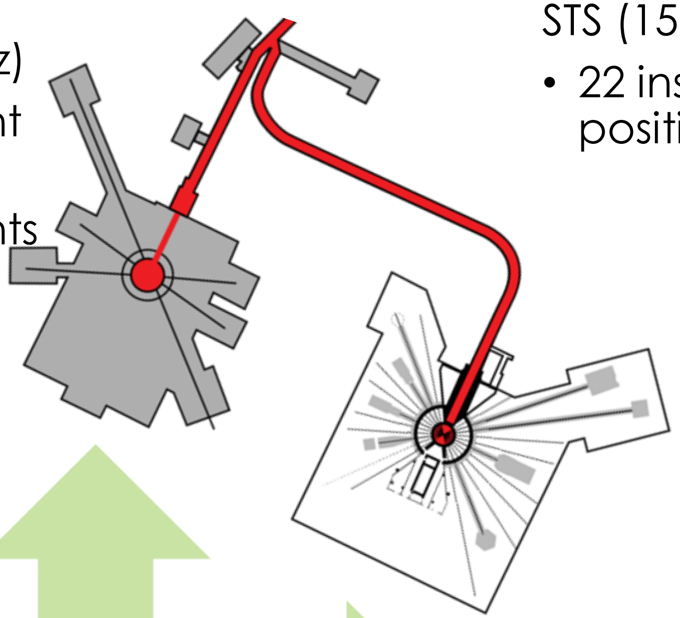
Future

FTS (3 out of 4 pulses at 60 Hz)

- 24 instrument positions
- 21 instruments built

STS (15 Hz)

- 22 instrument positions



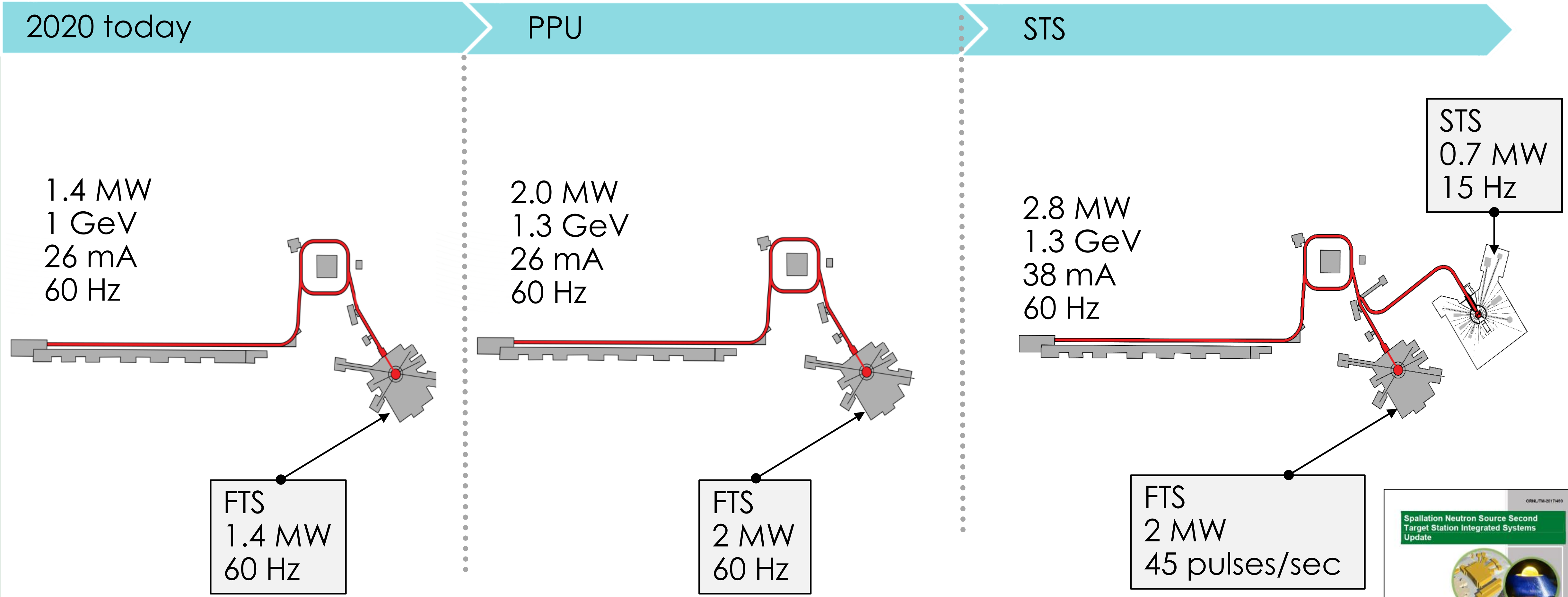
2 MW

0.7 MW

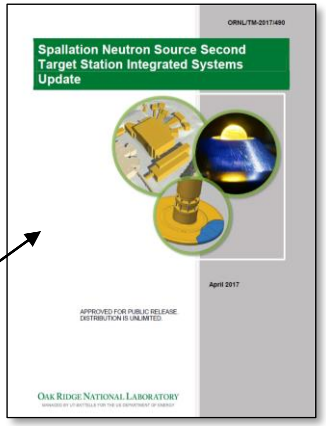
Accelerator after PPU

- Cold neutrons of unparalleled peak brightness (1.5×10^{15} n/s/cm^2/Å/sr at $\lambda = 3$ Å)
- Short pulses containing neutrons with broad ranges of usable wavelength or energy ($\Delta\lambda = 13.2$ Å at 15 Hz at 20 m distance from source)

A staged PPU and STS upgrade path



The choice of 15 Hz and 0.7 MW resulted from a detailed analysis of the STS design (reviewed by a panel of experts in 2017) and optimizes the performance of STS without impacting the performance of FTS.



Data reduction and data analysis

- Re-structuring proposed at DOE Review, July 2019
- Software development integrated into Research Software Engineering Group (CSMD), Jan. 2020
- Creation of the Computational Instrument Scientist position (6 of 8 positions filled), as part of instrument teams
- Data Reduction status:
  - Comprehensive tool kit for SANS released (drt-sans)
  - Current focus on residual stress (PyRS in acceptance testing), diffraction
  - Timeline for other techniques developed

Data reduction and data analysis (continued)

- Data Analysis working groups formed
- Presented at ACNS 2020 townhall meeting (7/16/2020)
- External advisory/review committee being formed
- “Road map” document to shape funding decisions

Technique	Coordinator / Lead
Powder Diffraction	Stuart Calder
Single Crystal Diffraction	Christina Hoffman
Engineering Diffraction	Ke An
Imaging	Jean Bilheux
Chemical Spectroscopy and Neutron Spin Echo	Timmy Ramirez-Cuesta
Reflectometry	Tim Charlton
Triple Axes and Direct Geometry Spectrometers	Garrett Granroth
Small Angle Scattering	Volker Urban

Mid-scale investments

- Competitive process (proposals)
- Selection by NSD Leadership team, with Science Initiative Coordinators, Sample Environment Steering Committees
- Typically ~$1M per year allocated from operating funds
- FY2019: $1.13M
  - In addition:
    - HYSPEC polarizer (~$750k)
    - MagREF fan analyzer repair (~$450k)
- FY2020: $1.4M

Examples of FY 2020 Mid-Scale Investments:

- Automated 10 kbar gas intensifier
- Dual Actuator Test System (load frame) for VULCAN
- Liquid Helium Autofill for HFIR instruments
- Cooling VTI for VISION
- He cold-flow system for TOPAZ
- Fluid control system for modes high presure
- 4-window tube furnace for VULCAN
- 7T Vanadium-tail magnet (POWGEN, NOMAD)
- Langmuir-Blodgett trough for membrane studies
- …

Instrument improvements and upgrades

- "Science Productivity" process for instrument improvements:
  - ~$10M/year
    (budget: FY2018: $10M; FY2019: $0M + $13M [VENUS]; FY2020: $7M)
  - Steering Committee: Group Leaders, Science Initiative Coordinators
  - On-going:
    - HB-3, TAX: Velocity Selector (FY 2020)
    - SNS 14T Magnet (FY 2020)
    - BL-7, VULCAN-X Phase 1 (FY 2020)
    - BL-3, SNAP: Beam Optics Upgrade (FY 2020)
    - HB-1A, FIE-TAX: Backend Upgrade (FY 2020/21)
    - BL-1B, NOMAD: Detectors (FY 2020/21)

Reviews of Instrument Suites

Aug. 10-11: Materials Engineering
Aug. 13-14: Diffraction
Aug. 18-19: SANS and Reflectometry
Sept. 17-18: Spectroscopy

- Requested by DOE (in addition to the Triennial Reviews)
- We see these reviews as advisory committee to help us prepare for the 2021 Triennial Review
  - The goal is not for us to look good, but to get your feedback
  - Not a competition between beamline, but helping each beamline
  - Assess the current capabilities and future needs
  - Comparison to beamlines at other facilities

Charge to committee

The committee is asked to consider the following:

- For each sub-panel, consider the status of the corresponding beamlines:
  - technical capabilities
  - Consider integration/overlaps within other SNS/HFIR instruments; comparison to instruments at other facilities
- The ability of each beamline to meet the needs of users for data collection, reduction, and analysis and future software planning
- The portfolio of science and business case for each instrument in the suite (e.g. demand; breadth of scientific use; overall impact)

Charge to committee (continued)

- The future development and use of the suite of instruments
- Other developments to enhance the capacity or effectiveness of these instruments
- Strategic visions of the beamlines, alignment with ORNL and DOE missions and effectiveness of process to implement vision
- Any other comments the panel wishes to make to the NScD Associate Laboratory Director

Suite Checklist

1. Scientific Mission and Impact
   - How do the performance and capabilities of the instrument suite compare to other neutron sources?
   - Are the plans for future instrument and technique improvements aligned with future science directions?

2. Leveraging of specific SNS/HFIR characteristics

3. Clearly articulated vision that prioritizes future investments and emphasizes complementarities/synergies within the suite

4. Leveraging of NTD efforts and other ORNL resources to enhance the impact of the suite

5. Leveraging expertise of instrument users including NSD staff and external researchers to improve the impact of the suite

6. Adequacy and reliability of software, sample environment and ancillary equipment

7. Overall comments and recommendations on suites

Individual Instrument Checklist

1. Instrument Productivity
2. Effectiveness of beam time use
3. General User program quality
4. Instrument upgrades
   – Fully benefiting from prior upgrade investments
   – Future development plan
5. Summary Strength/Weakness/Opportunities/Threats discussion; recommended actions including upgrades/improvements, continued operation, a re-review *before* three years, or termination/decommissioning/repurposing.

Thursday, Sept. 17

8:30–8:50 am	Welcome (Paul Langan)		Microsoft Teams Link Conference ID: 990 971 229#
8:50–9:20 am	Neutron Scattering Division Outlook & Strategy (Hans Christen)		
9:20–9:50 am	Spectroscopy Overview & Strategy (Mark Lumsden)		
9:50–10:15 am	Break		
10:15 am–12:05 pm	**Parallel Beam line presentations**		
	Direct Geometry ***Microsoft Teams Link*** *Conference ID: 288 086 343#*	***Triple-Axis*** ***Microsoft Teams Link*** *Conference ID: 324 053 44#*	***Chemical Spectroscopy*** ***Microsoft Teams Link*** *Conference ID: 893 804 295#*
10:15–10:25 am	Team overview (Doug Abernathy)	Team overview (Jaime Fernandez-Baca)	Team overview (Timmy Ramirez-Cuesta)
10:25–10:50 am	CNCS (Daniel Pajerowski)	CTAX (Tao Hong)	BASIS (Eugene Mamontov)
10:50-11:15 am	HYSPEC (Barry Winn)	HB-1 (Masa Matsuda)	NSE (Laura Stingaciu)
11:15–11:40 am	SEQUOIA (Matt Stone)	HB-1A (Adam Aczel)	VISION (Luke Daemen)
11:40 am–12:05 pm	ARCS (Doug Abernathy)	HB-3 (Songxue Chi)	
12:05–1:00 pm	***LUNCH***		
1:00-1:30 pm	Direct Geometry / Triple-axis software (A. Savici) Microsoft Teams Link Conference ID: 163 506 91#		Chemical spectroscopy software (YQ Cheng) Microsoft Teams Link Conference ID: 100 797 100#
1:30 pm -	Committee work time and report writing • Direct Geometry: Microsoft Teams Link; Conference ID: 603 993 950# • Chemical Spectroscopy: Microsoft Teams Link; Conference ID: 422 845 8# • Triple-Axis: Microsoft Teams Link; Conference ID: 324 053 44#		

Friday, Sept. 18

9:00–9:30 am	Committee recap and Q&A (GL and TLs): Microsoft Teams Link; Conference ID: 151 087 587#		
9:30–11:30 am	Meet with Direct Geometry Team members Microsoft Teams Link Conference ID: 962 280 998#	Meet with Triple-Axis Team members Microsoft Teams Link Conference ID: 150 682 173#	Meet with Chemical Spectroscopy Team members Microsoft Teams Link Conference ID: 102 449 122#
11:30 am-12:30 pm	Committee work time and report writing • Direct Geometry: Microsoft Teams Link; Conference ID: 517 932 137# • Chemical Spectroscopy: Microsoft Teams Link; Conference ID: 847 467 074# • Triple-Axis: Microsoft Teams Link; Conference ID: 152 490 559#		
12:30-1:30 pm	Lunch		
1:30–2:30 pm	Committee Verbal Report and Recommendations (DD, GL, TLs, instrument teams) Microsoft Teams Link Conference ID: 401 605 059#		
2:30 p.m.	Adjourn		

https://conference.sns.gov/event/242 PW: nsdbr20

On standby: Georg Ehlers, Neutron Technologies Division

Presentations and Q&A will be recorded for my own benefit (scheduling conflicts)

Thank you!