NIST CENTER FOR NEUTRON RESEARCH

Neutron Sources and the NCNR User Program

Brian Kirby

Group Leader, Research Facility Operations

NIST Center for Neutron Research

ISRD-RCN Workshop: Exploring Dynamic Properties of Earth and Planetary Materials Using Neutron Scattering and Imaging

July 25, 2023

NIST Center for Neutron Research

Our Mission

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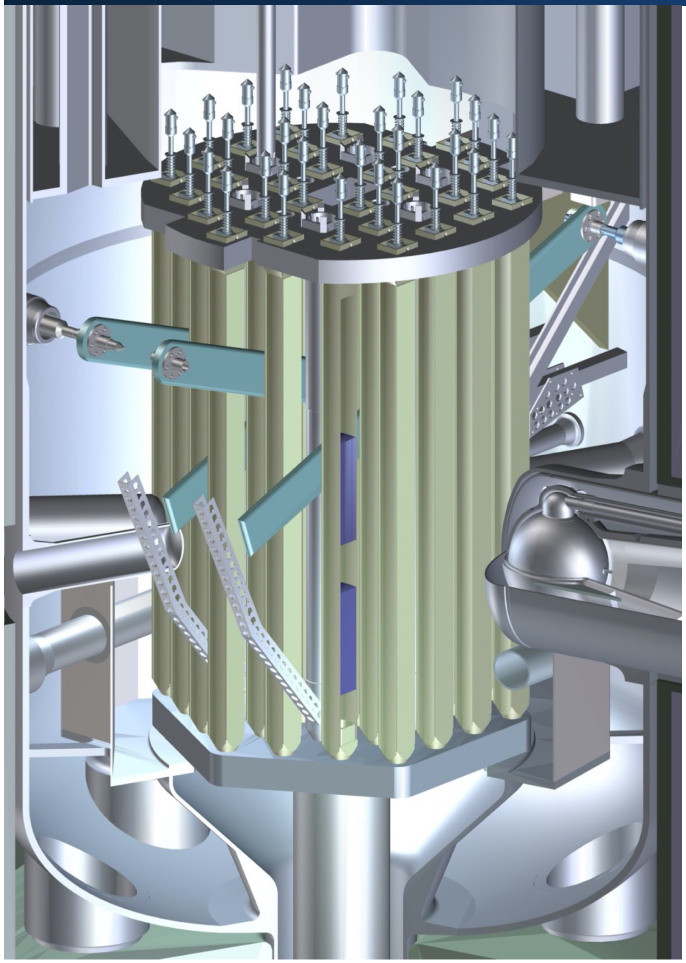
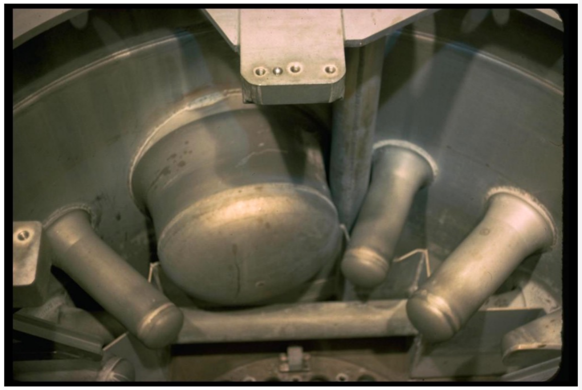
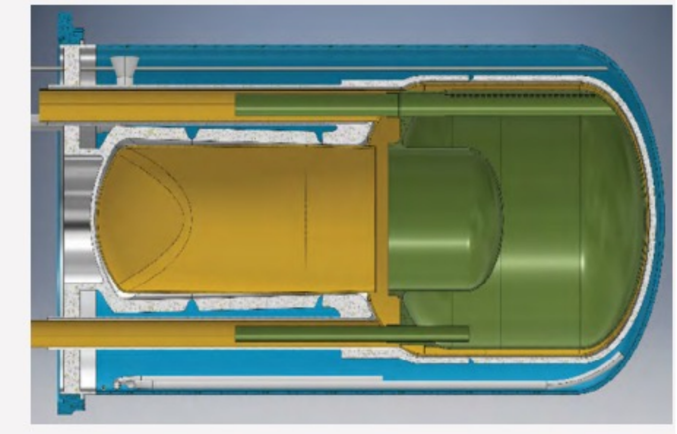
NCNR is a national user facility that provides advanced neutron measurement capabilities to meet the needs of U.S. researchers from industry, academia, and government agencies.

NIST Bureau of Standards Reactor



- Online in 1967
- 20 MW, D_2O moderated
- Research, not power
- 24h operation, 200+ days/year
- Currently operating for low power testing





Experimental Area

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Experimental Area

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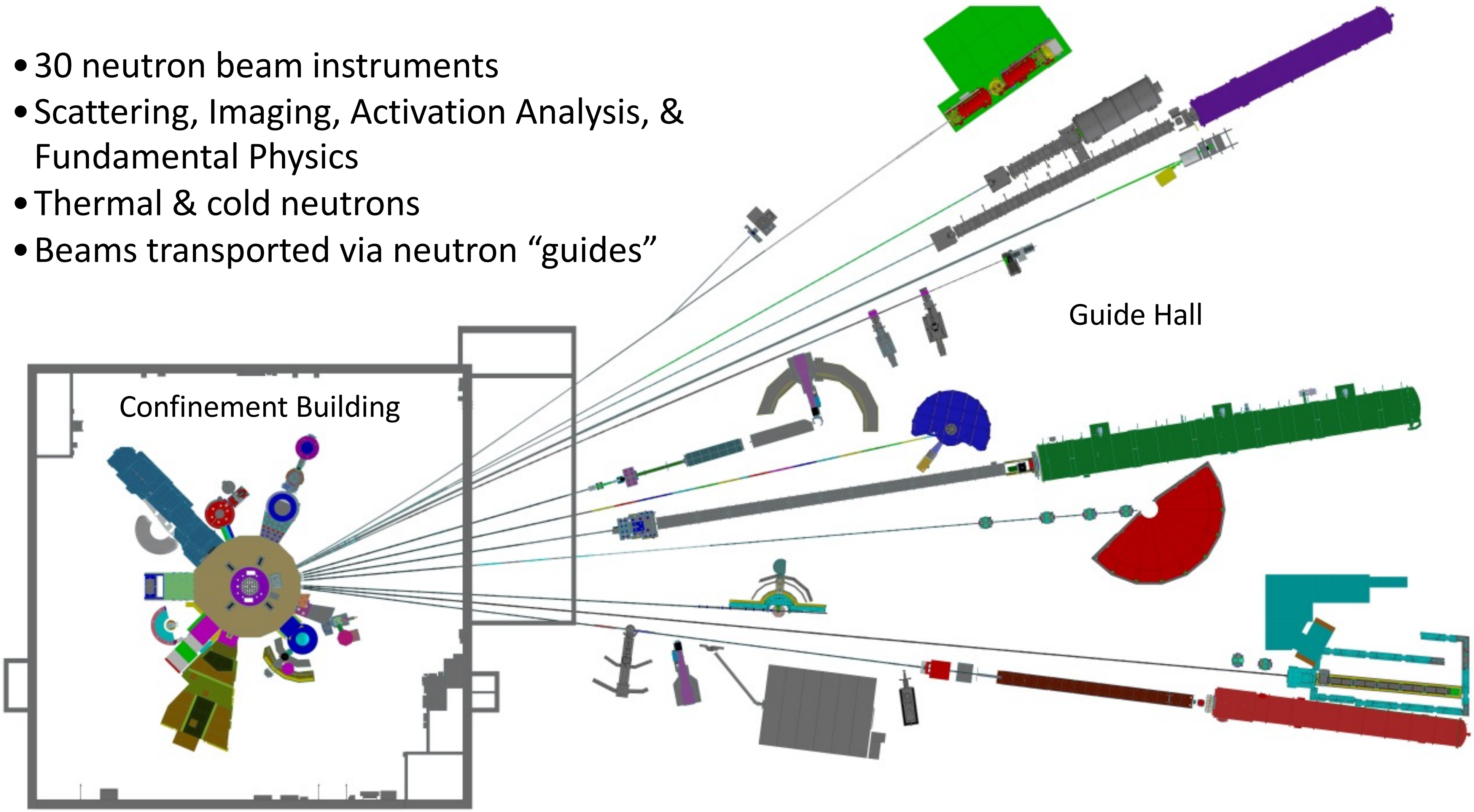
- 30 neutron beam instruments
- Scattering, Imaging, Activation Analysis, & Fundamental Physics
- Thermal & cold neutrons
- Beams transported via neutron “guides”



User Program

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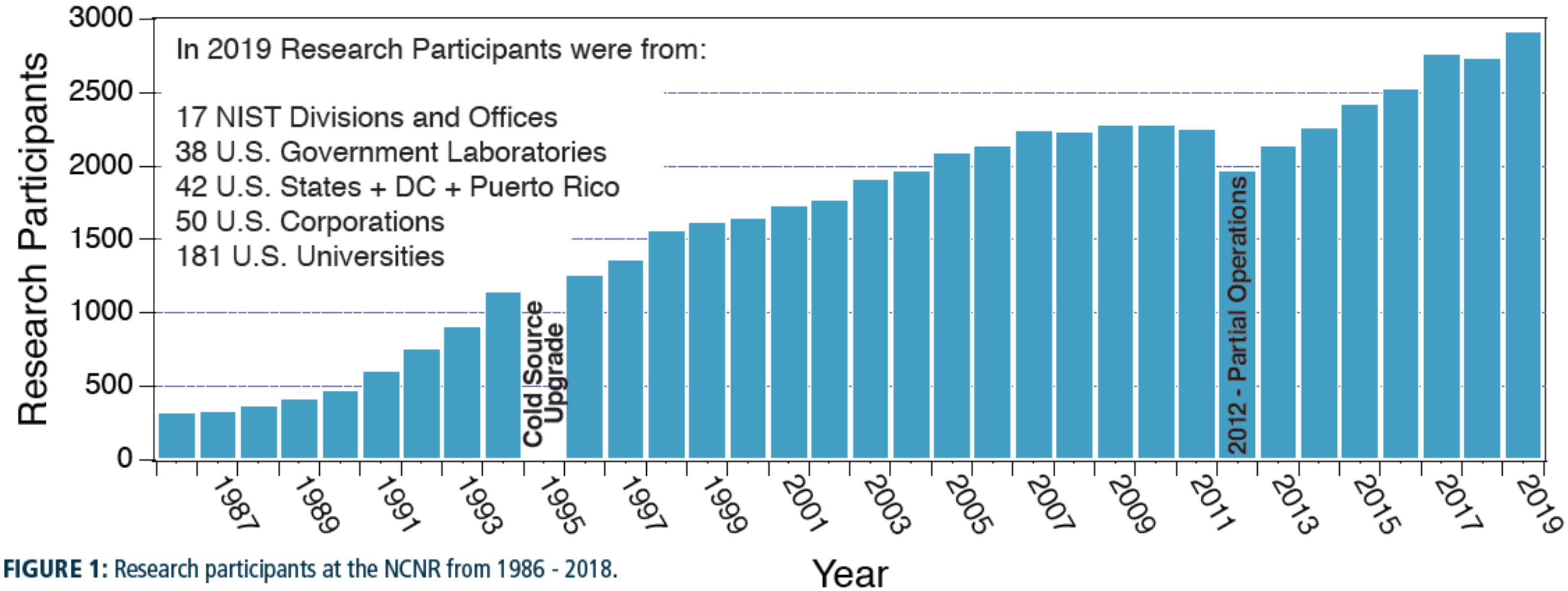

FIGURE 1: Research participants at the NCNR from 1986 - 2018.

- Neutron measurement capabilities require facility-scale infrastructure
- Only 2 sites in the U.S., NIST-Gaithersburg & Oak Ridge National Lab
- NCNR serves U.S. industry, academia, and government researchers
- Access: General User, Collaborative, Industrial Consortium, Proprietery
- About 2500 research participants, 300 publications per year

CHRNS

Center for High Resolution Neutron Scattering
A partnership between the National Science Foundation and NIST

OBJECTIVES:

- Develop & operate neutron scattering instrumentation, with broad application in materials research, for use by the general scientific community
- Promote the effective use of the CHRNS instruments by having an identifiable staff whose primary function is to assist users
- Conduct research that advances the capabilities and utilization of CHRNS facilities
- Contribute human resources development through educational and outreach efforts

Maximizing access for the scientific community to transformative neutron scattering instrumentation

CHRNS

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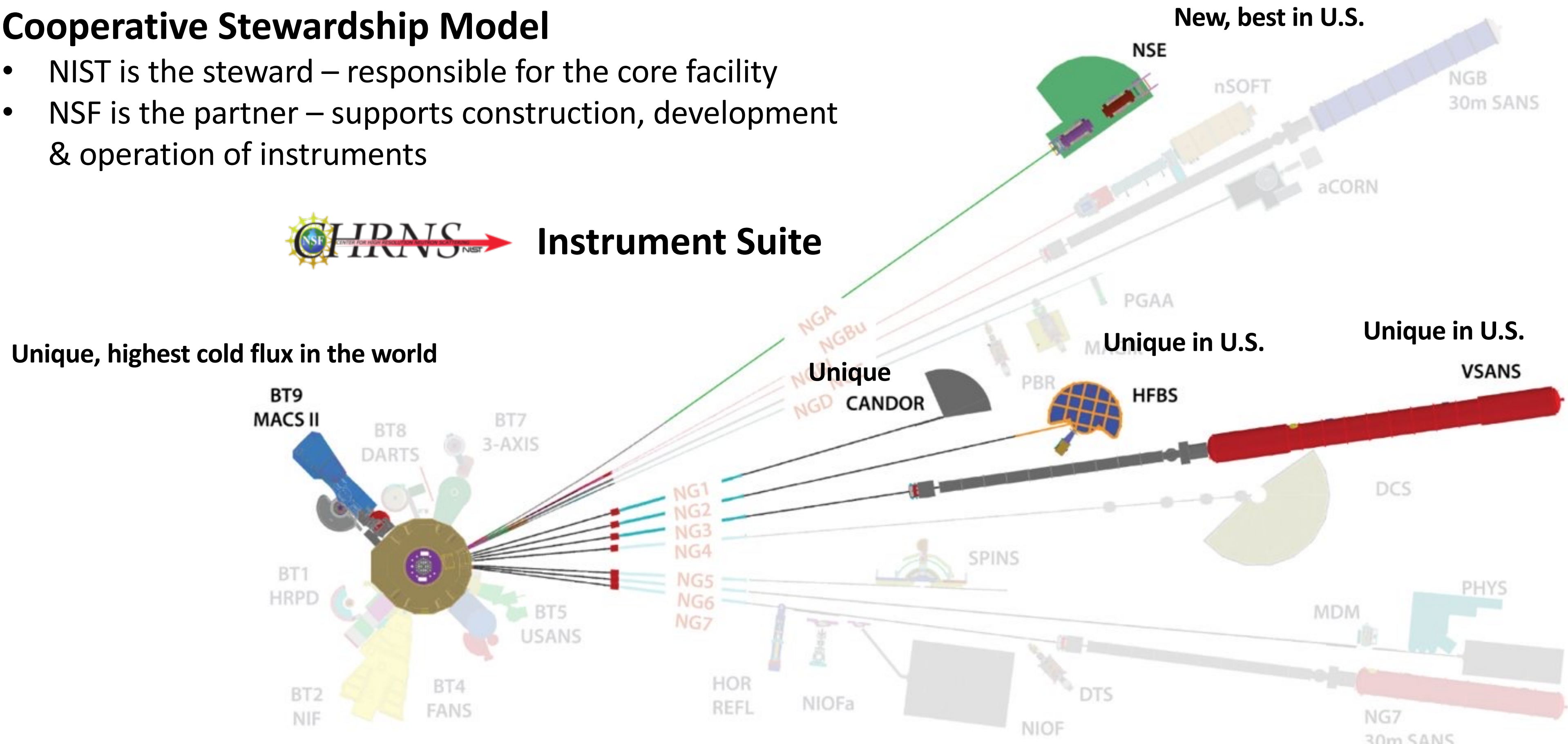
Cooperative Stewardship Model

- NIST is the steward – responsible for the core facility
- NSF is the partner – supports construction, development & operation of instruments

CHRNS → **Instrument Suite**



NSF Midscale Research Infractructure - NSE II

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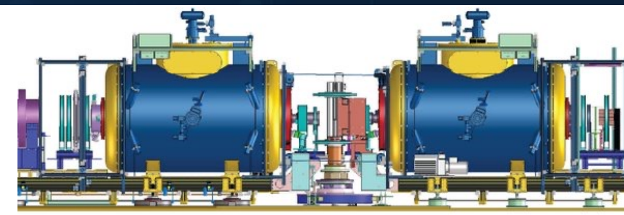
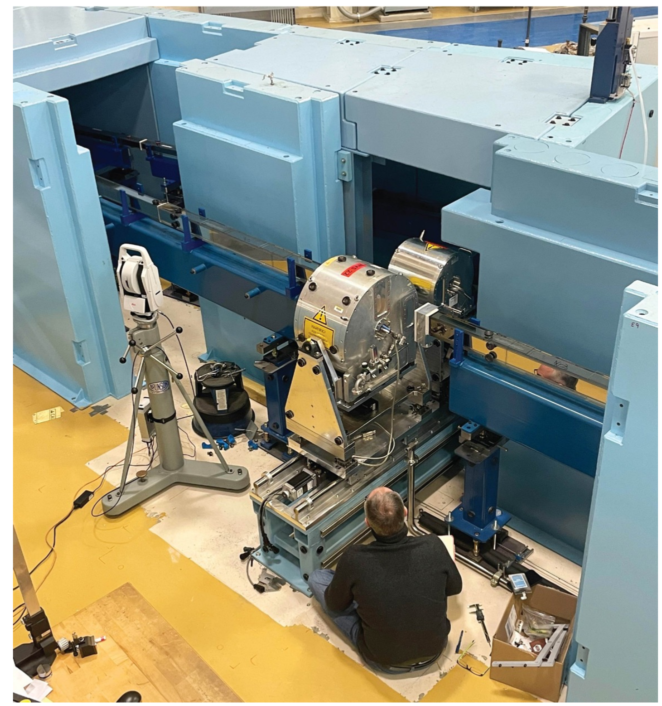
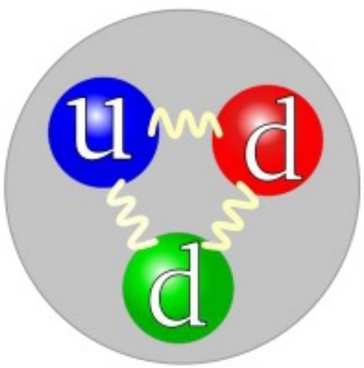




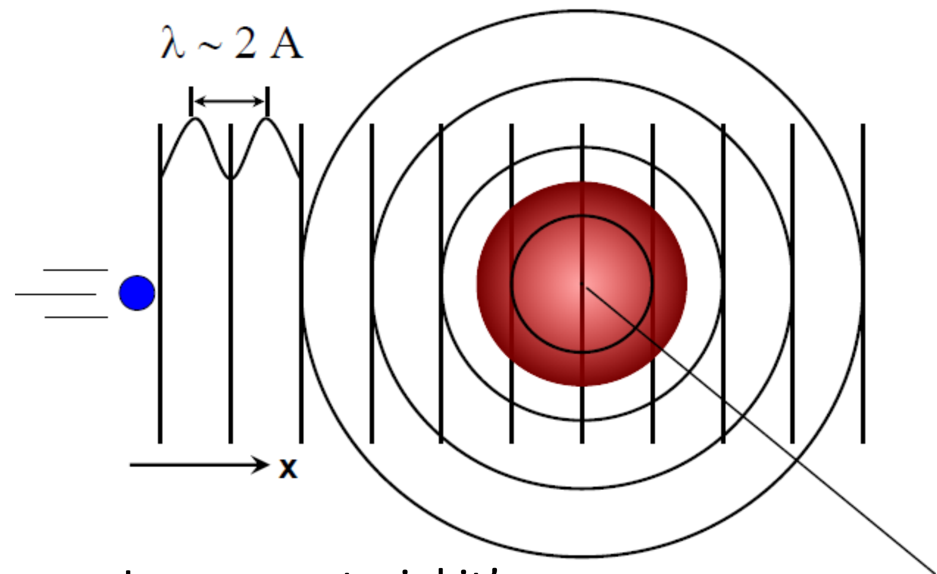
- NIST & UDel Center for Neutron Science
- Funded by National Science Foundation
- All components in-house
- On track for hot commissioning in 2023
- Only NSE in North America under construction
- 10x data rate, extended dynamic range

Neutron Measurements

A Free Neutron



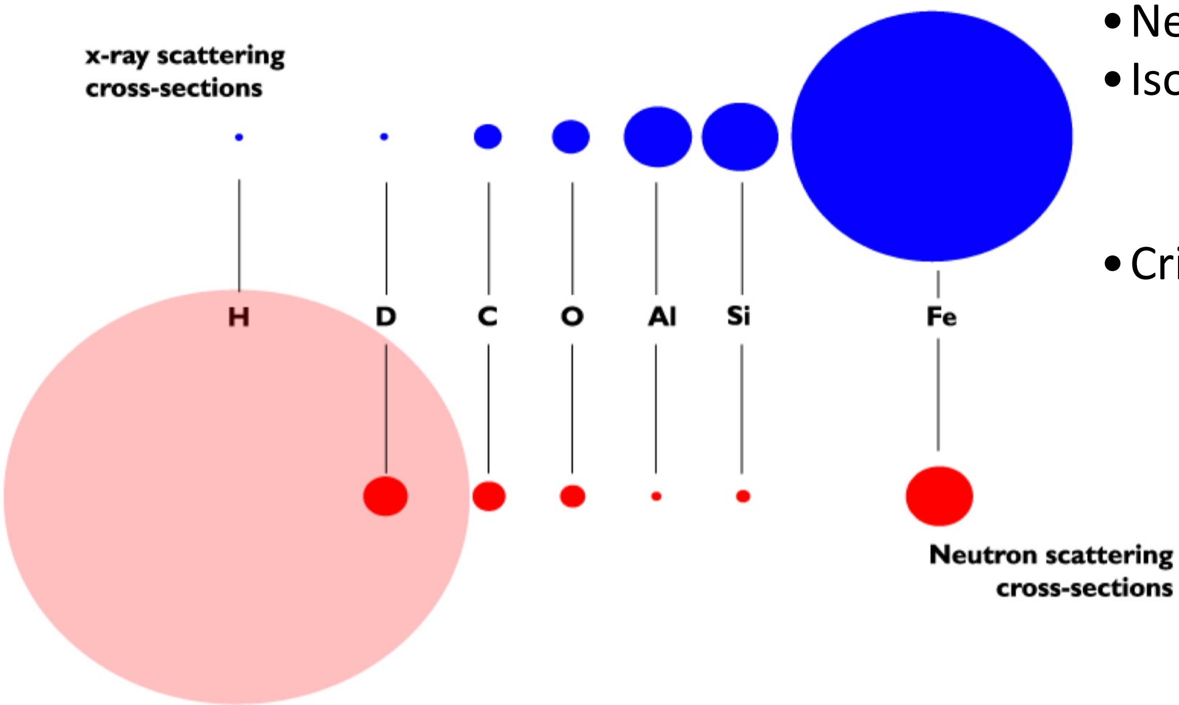
$m_n = 1.675 \times 10^{-27}$ kg
Q = 0
S = ½ ħ
$\mu_n = -1.913\ \mu_N$



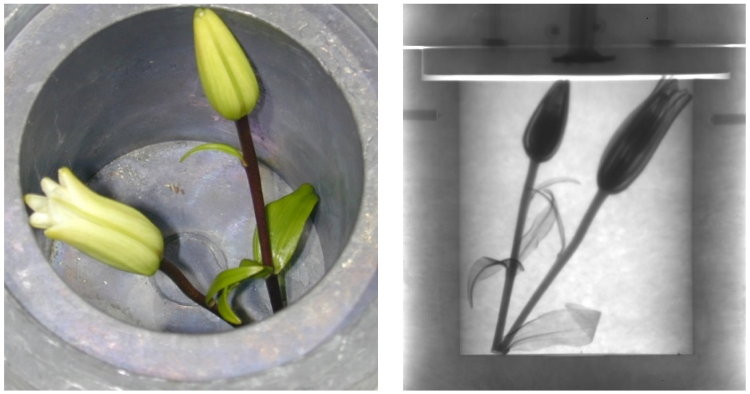
- No Charge
- Interacts with nuclei
  - Diffraction, absorption, activation
- Large magnetic moment
  - Interacts with magnetic fields

- In your material it's a wave
  - Energy, velocity, wavelength…
  - Interferes with itself
- Large magnetic moment
  - Interacts with magnetic fields

Nuclear Sensitivity

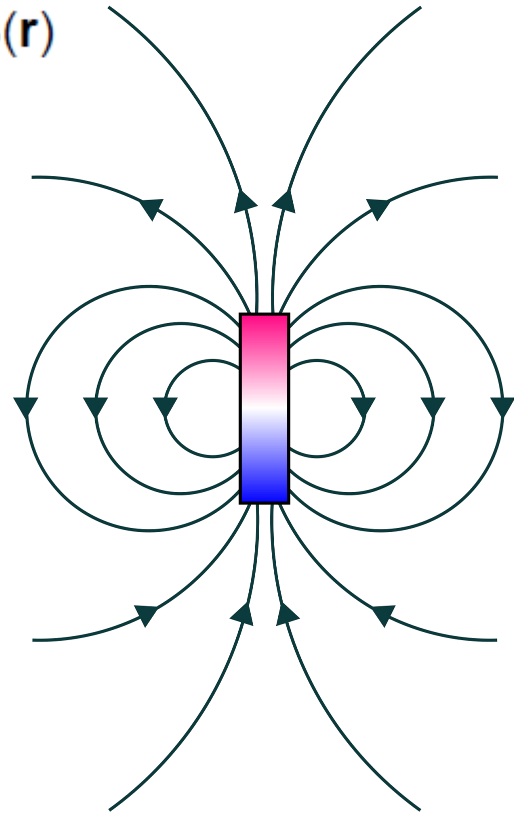


- Most probes see charge
- Neutrons sensitive to light elements
- Isotopic control of contrast
  - No change in chemical properties
  - e.g., replace H with deuterium
- Critical tool for soft matter

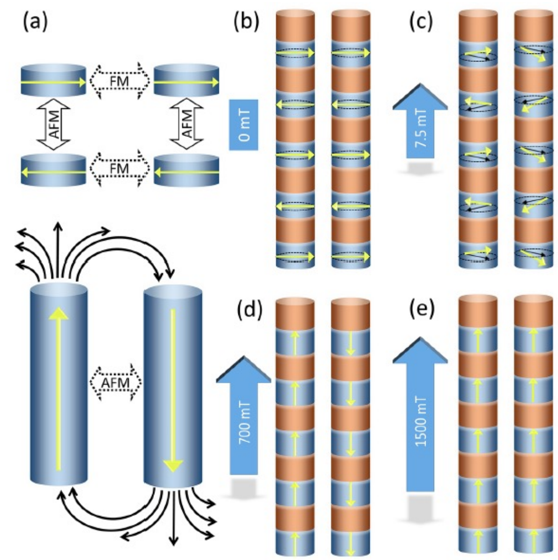


Magnetic Sensitivity

$$V_M(\mathbf{r}) = -\mu_n \cdot \mathbf{B}(\mathbf{r})$$

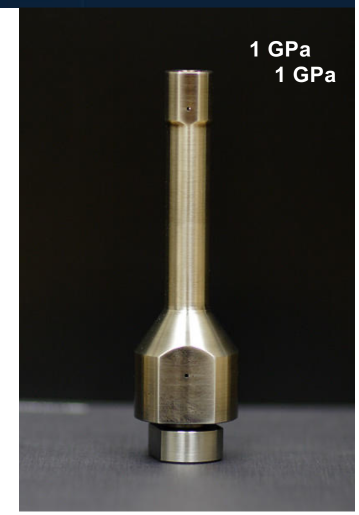


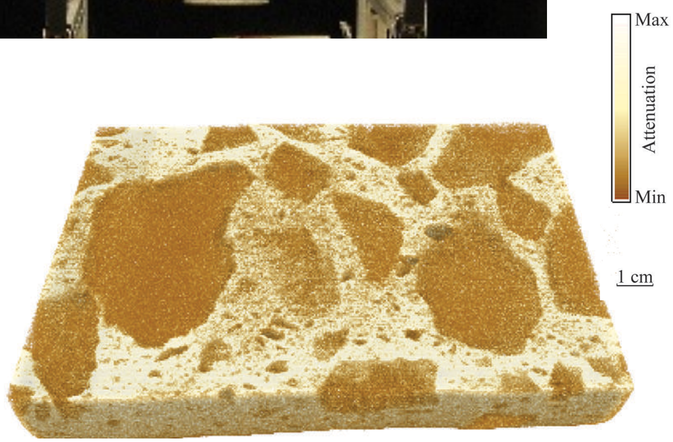
- Direct interaction with **B**
  - m, M, D in real units
- Comparable to nuclear interaction
- Indispensable for magnetic structure

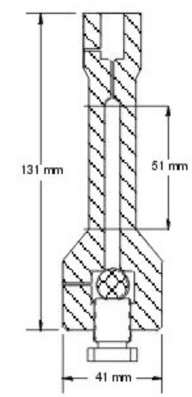


Weakly Interacting

- Interaction is weak
- Interpretation is easy
- Windows are easy
- Exotic sample environments
  - mK – kK, 15 T, 2.5 GPa
  - E-field, gas loading…
- See deep inside samples







Neutron Diffraction

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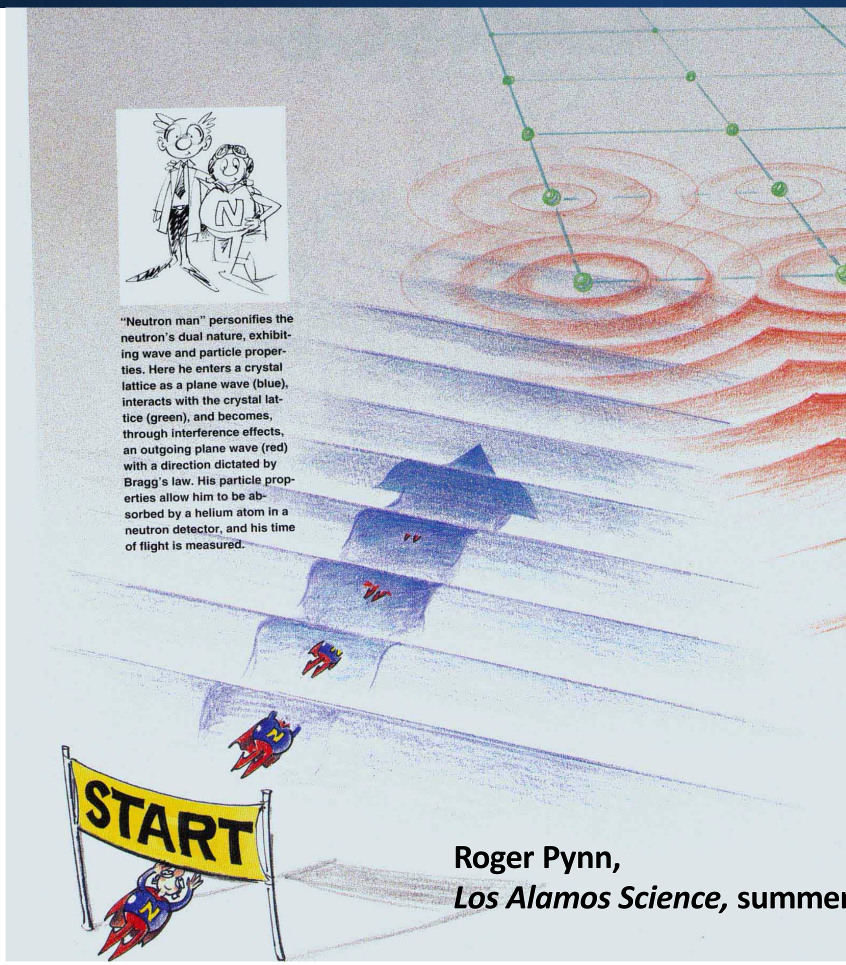
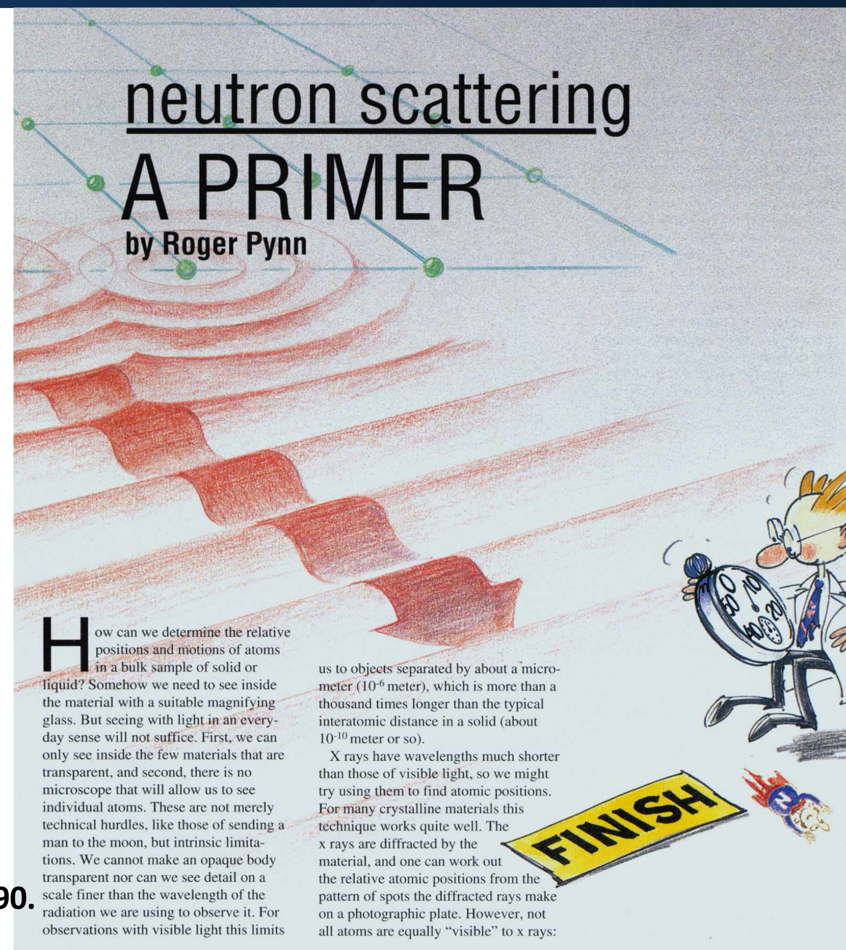


"Neutron man" personifies the neutron's dual nature, exhibiting wave and particle properties. Here he enters a crystal lattice as a plane wave (blue), interacts with the crystal lattice (green), and becomes, through interference effects, an outgoing plane wave (red) with a direction dictated by Bragg's law. His particle properties allow him to be absorbed by a helium atom in a neutron detector, and his time of flight is measured.



neutron scattering

A PRIMER

by Roger Pynn

How can we determine the relative positions and motions of atoms in a bulk sample of solid or liquid? Somehow we need to see inside the material with a suitable magnifying glass. But seeing with light in an everyday sense will not suffice. First, we can only see inside the few materials that are transparent, and second, there is no microscope that will allow us to see individual atoms. These are not merely technical hurdles, like those of sending a man to the moon, but intrinsic limitations. We cannot make an opaque body transparent nor can we see detail on a scale finer than the wavelength of the radiation we are using to observe it. For observations with visible light this limits us to objects separated by about a micrometer (10^{-6} meter), which is more than a thousand times longer than the typical interatomic distance in a solid (about 10^{-10} meter or so).

X rays have wavelengths much shorter than those of visible light, so we might try using them to find atomic positions. For many crystalline materials this technique works quite well. The x rays are diffracted by the material, and one can work out the relative atomic positions from the pattern of spots the diffracted rays make on a photographic plate. However, not all atoms are equally "visible" to x rays:

Roger Pynn,
***Los Alamos Science,* summer 1990.**

Neutron Diffraction

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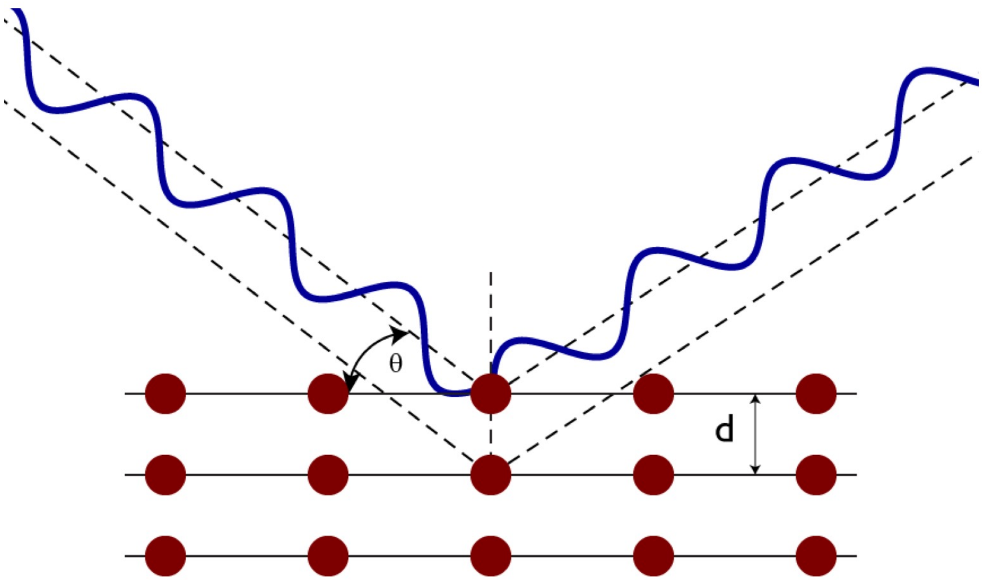
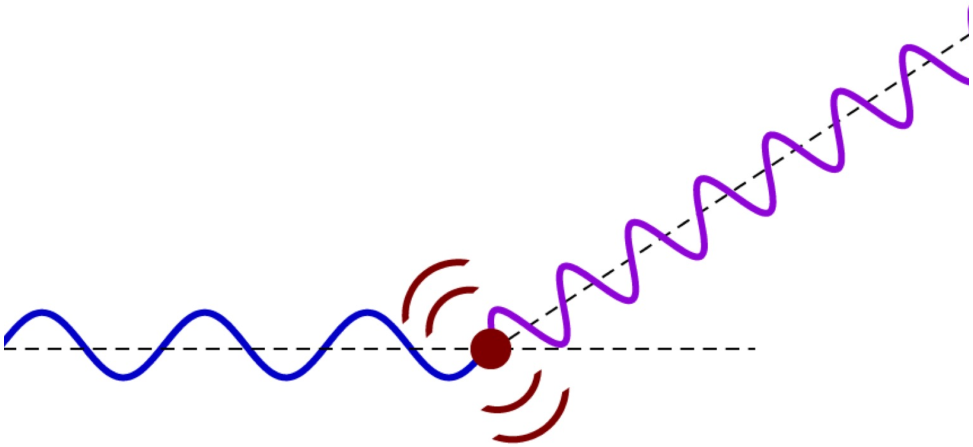
λ ~ interatomic spacing

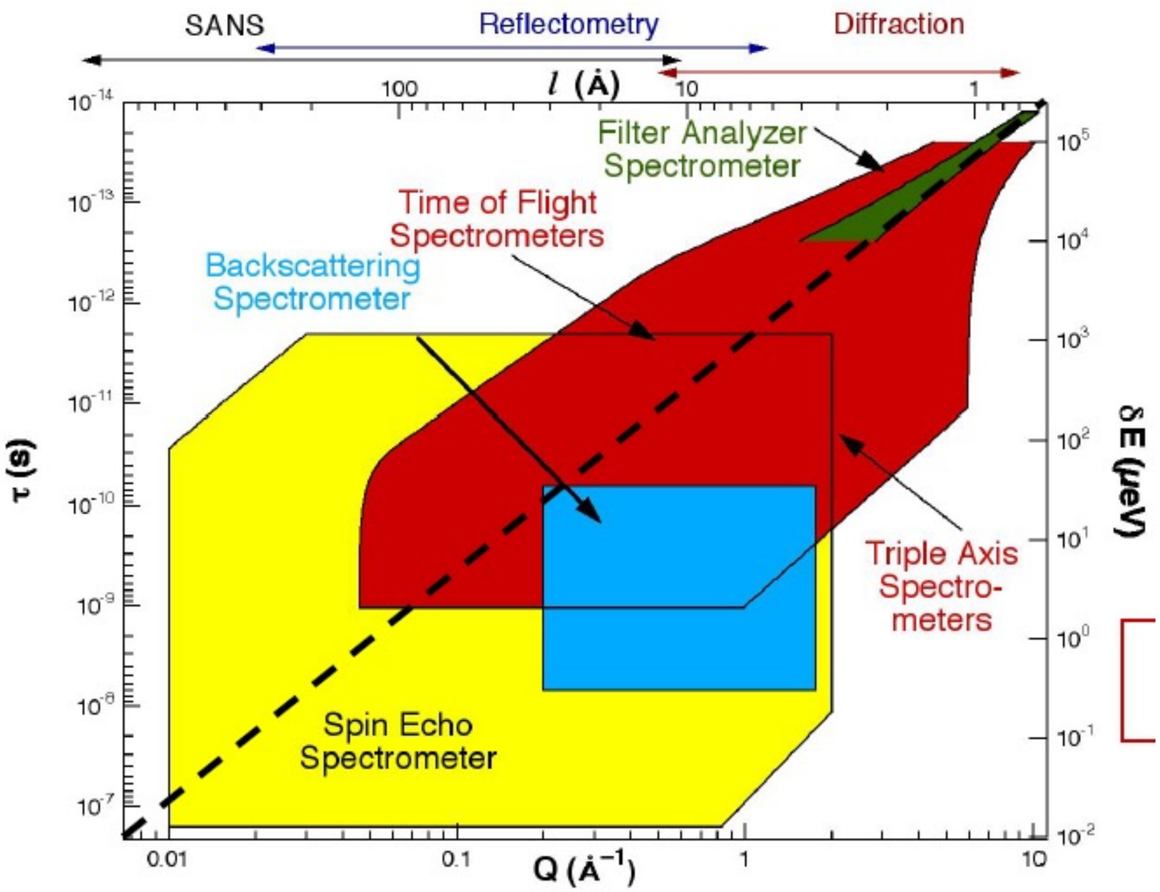


E ~ atomic motion

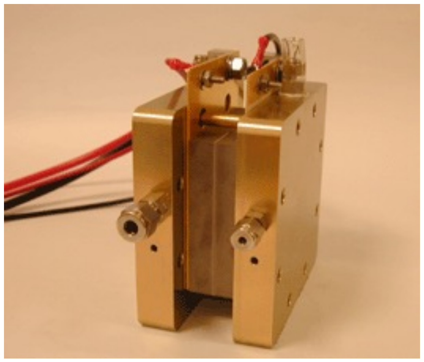


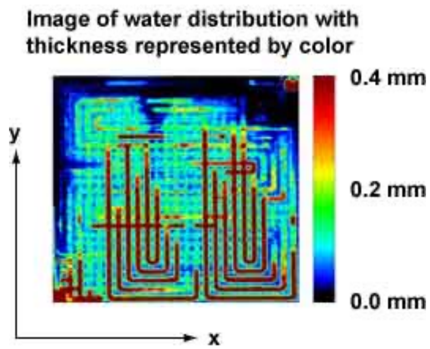
- Where atoms are
- How atoms move
- Highly specialized instruments

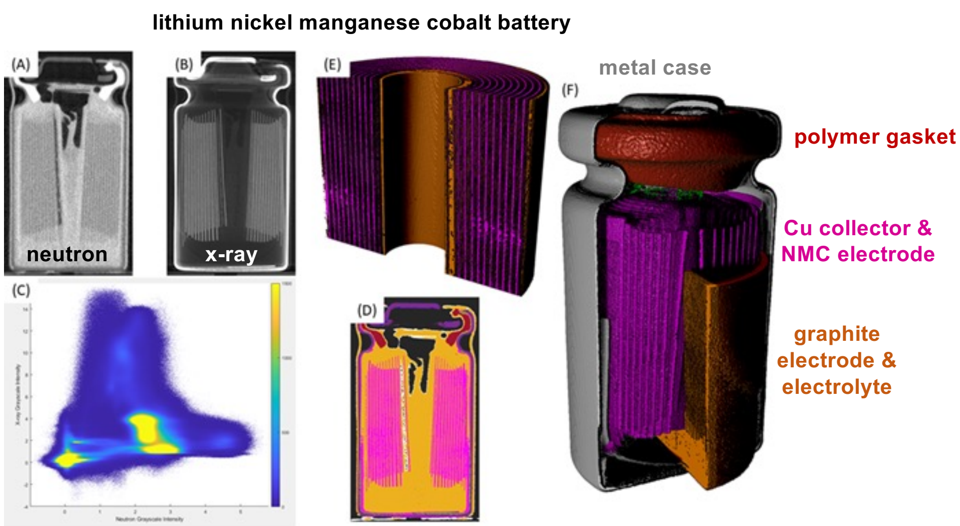
Scattering Instrumetation



Neutron Imaging







- Powerful, rapidly developing, & industrially relevant technique
- Particularly relevant for geology
- Thermal & cold imaging at NCNR
- Neutrons and x-rays available (NeXT)
- You'll hear much more this week

Activation Analysis

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Glass SRMs for forensic science

- Neutron activation analysis
  - High sensitivity elemental composition (µg / g or better)
  - Semiconductor doping, radiopharma, forensics
- <u>Critical for Standard Reference Material (SRM) Certification</u>
- Industry, academia, & government use NIST SRMs to facilitate commerce and advance R&D
- 80% of NIST SRMs are chemical composition standards
- Independent measurements required for verification
  - Nuclear instead of chemical sensitivity
  - Used for over 300 Reports of Analysis for SRM certification
  - Not commonly available for other standards organizations
- Clear mission need for NIST

Science Examples

CO_2 capture with MOFs

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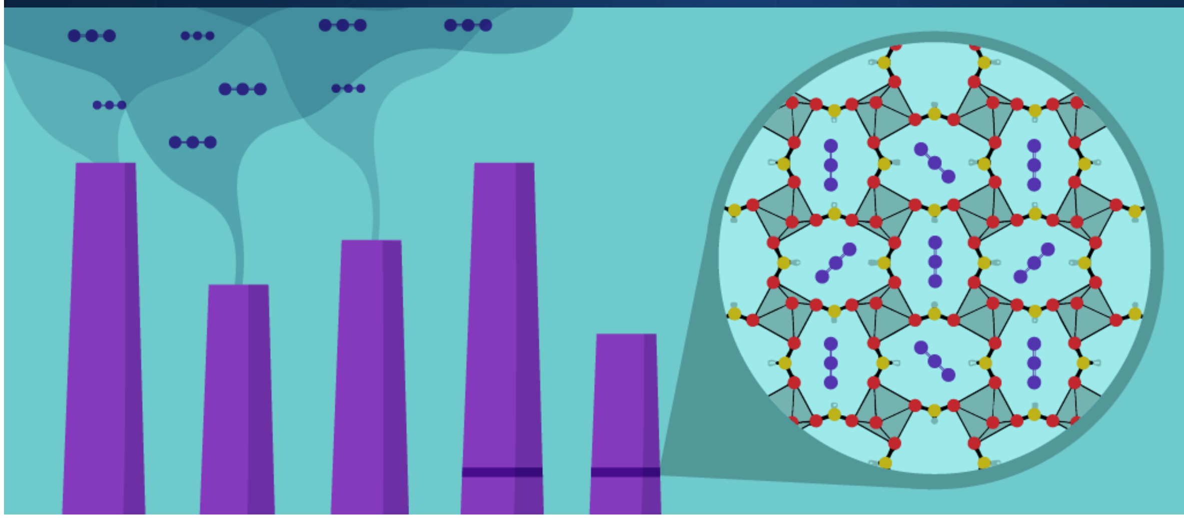
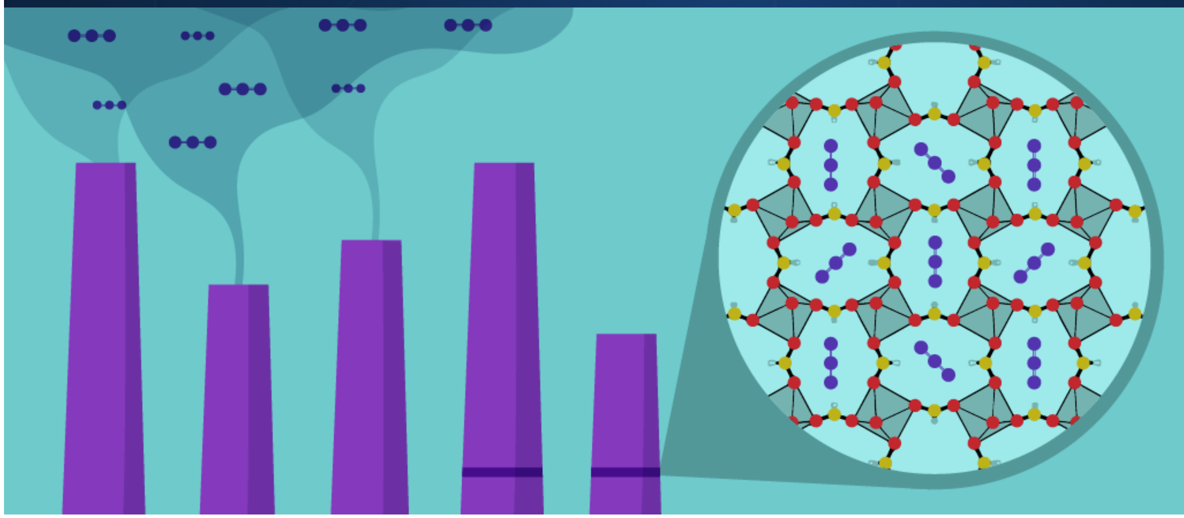


Hayden Evans & Craig Brown
NIST, Nat. U. Singapore, Singapore ASTR, U. Del, UCSB
Science Advances, 2022, 10.1126/sciadv.ade1473

CO_2 capture with MOFs



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- Metal organic framework: Cage for filtering & separating organic materials
- Aluminum formate (ALF), $AlC_3H_3O_6$
    - Cage is just big enough for CO_2, just small enough to exclude nitrogen
    - Good for CO_2 emissions at coal-fired power plants (30% of global CO_2)
    - 100x less expensive than other materials

CO_2 capture with MOFs

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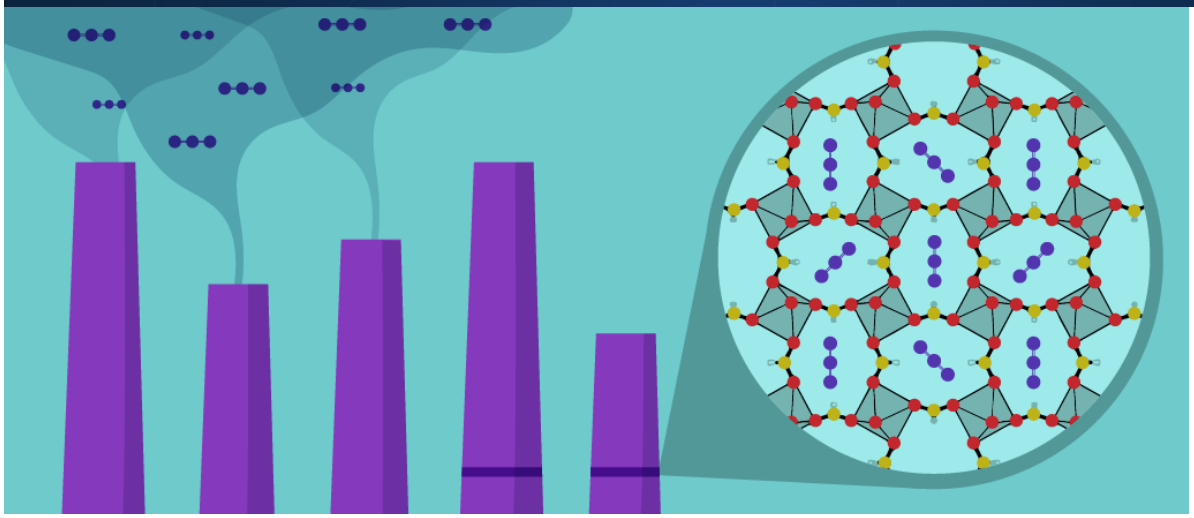

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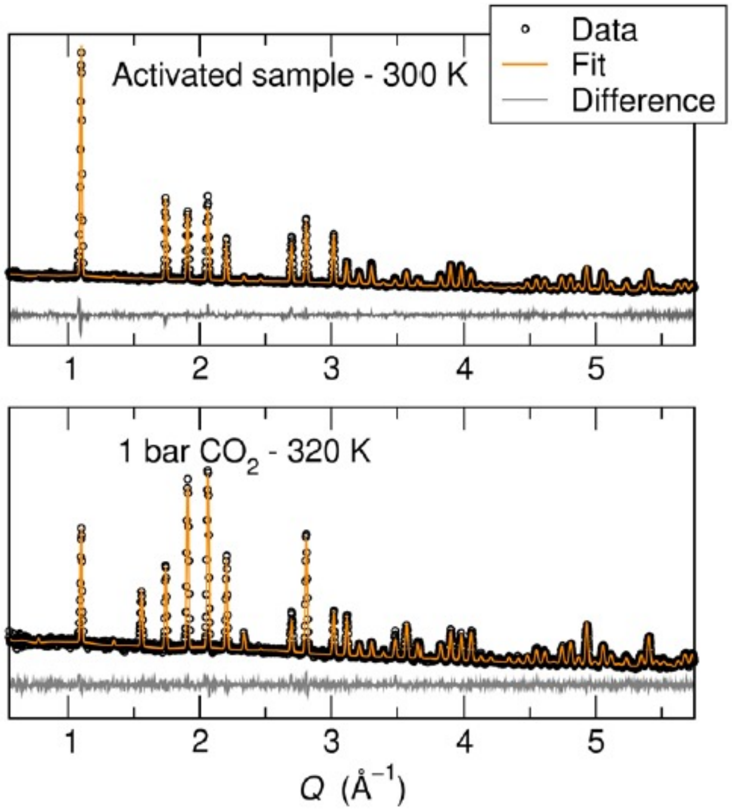

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  - Cage is just big enough for CO_2, just small enough to exclude nitrogen
  - Good for CO_2 emissions at coal-fired power plants (30% of global CO_2)
  - 100x less expensive than other materials
- Neutron powder diffraction reveals atomic structure as a function of temperature & pressure
- Also good for hydrogen, patent application submitted

Color Filter Gel

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Yun Liu
NIST & University of Delaware
Nature Communications, 2022, 10.1038/s41467-022-31020-0

Color Filter Gel

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NIST & University of Delaware
Nature Communications, 2022, *10.1038/s41467-022-31020-0*

- Optical properties ↔ periodic structures
- SeedGel: Temp-dependent color filter
- Water, solvents, and silica nanoparticles

Color Filter Gel

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Yun Liu
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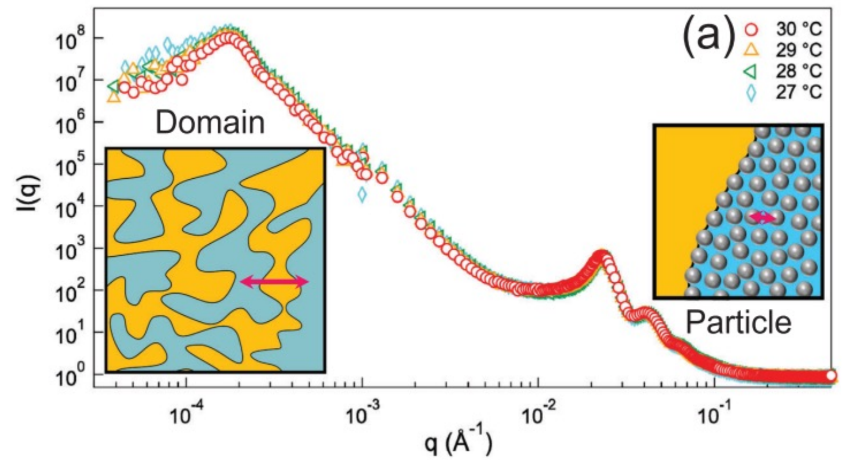
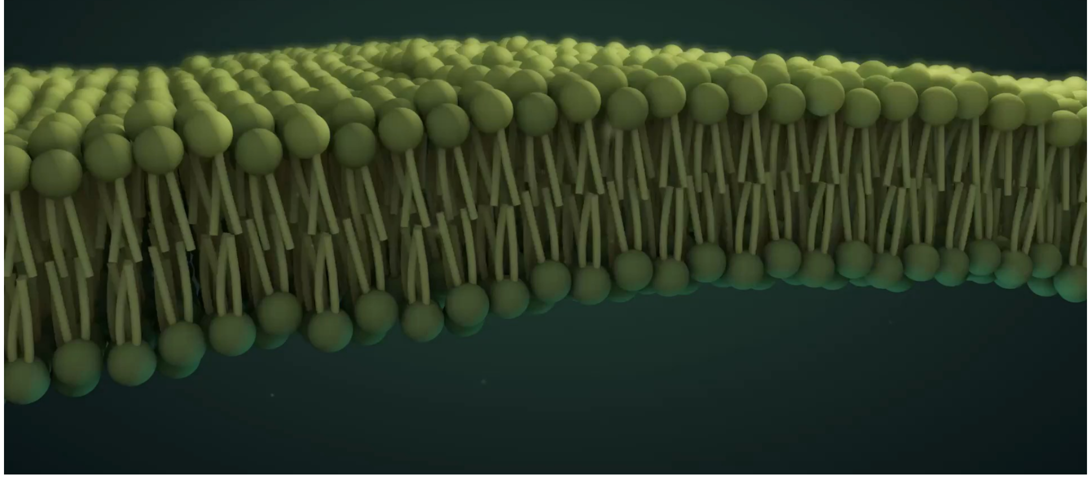
Nature Communications, 2022, 10.1038/s41467-022-31020-0

- Optical properties ↔ periodic structures
- SeedGel: Temp-dependent color filter
- Water, solvents, and silica nanoparticles
- SANS: microscopic structure T-independent
- µm-sized bicontinuous domains
- Color driven by µ-phase sep of binary solvents



Cell Membrane Viscosity

Michihiro Nagao & Liz Kelley
NIST, UMD, UDel, Kyoto U., JSRRI, J-PARC, UT-Knoxville
PRL, 2021, 10.1103/PhysRevLett.127.078102



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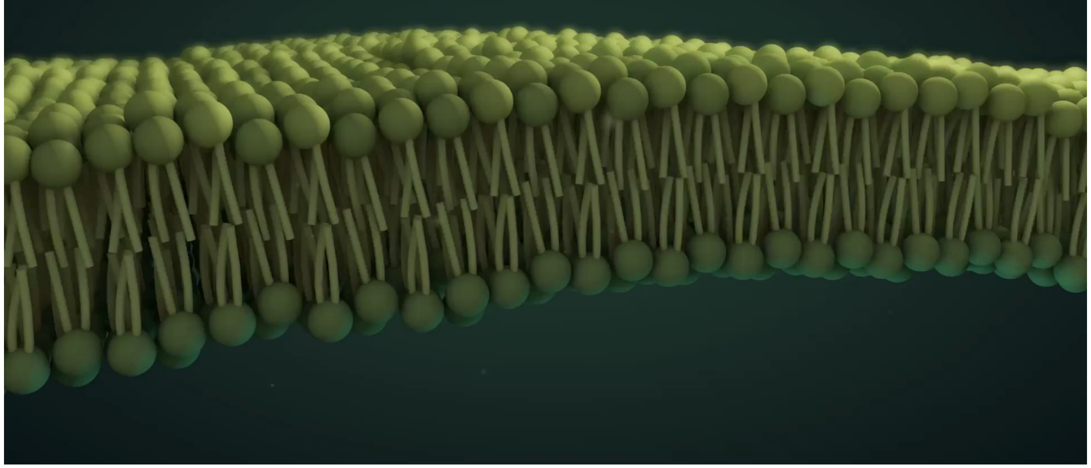

Cell membranes

- Fatty lipid molecules that encapsulate cells
- Membrane proteins & channels are gates to the cell interior
- Not solid – 2 molecule thick, viscosity determines functionality
- No good conventional probe for lipid motion, particularly at 2D

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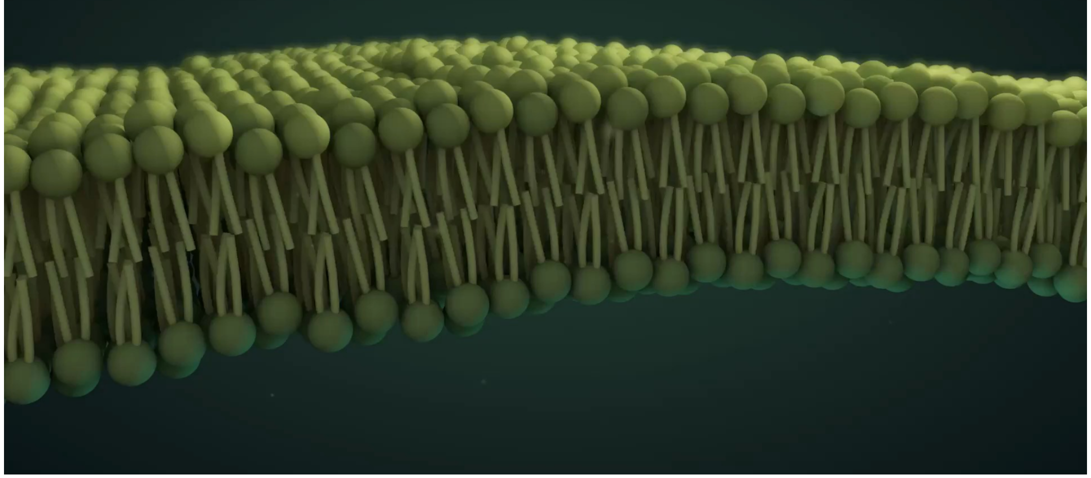

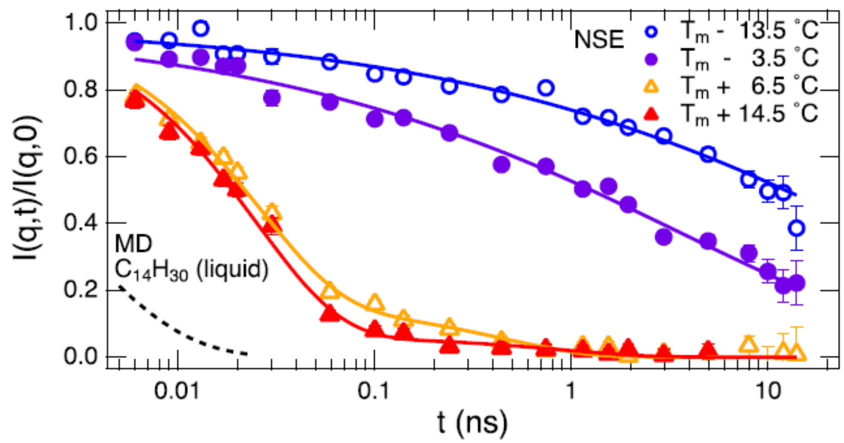

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Neutron Spin Echo

- Maps collective motion onto neutron polarization
- Low energy excitations (µs-ps, neV-0.1 meV)
- Normalized intermediate scattering function: spatial FT of the space-time correlation function near gel transition
- Connected timesceale of lipid motion to viscosity
- Being 2D slows motions & increases interactions – higher viscosity than in 3D
- Directly links acyl tail dynamics to cell function – pathway to "membrane lipid therapies"

Neutron Sources

Research Reactors

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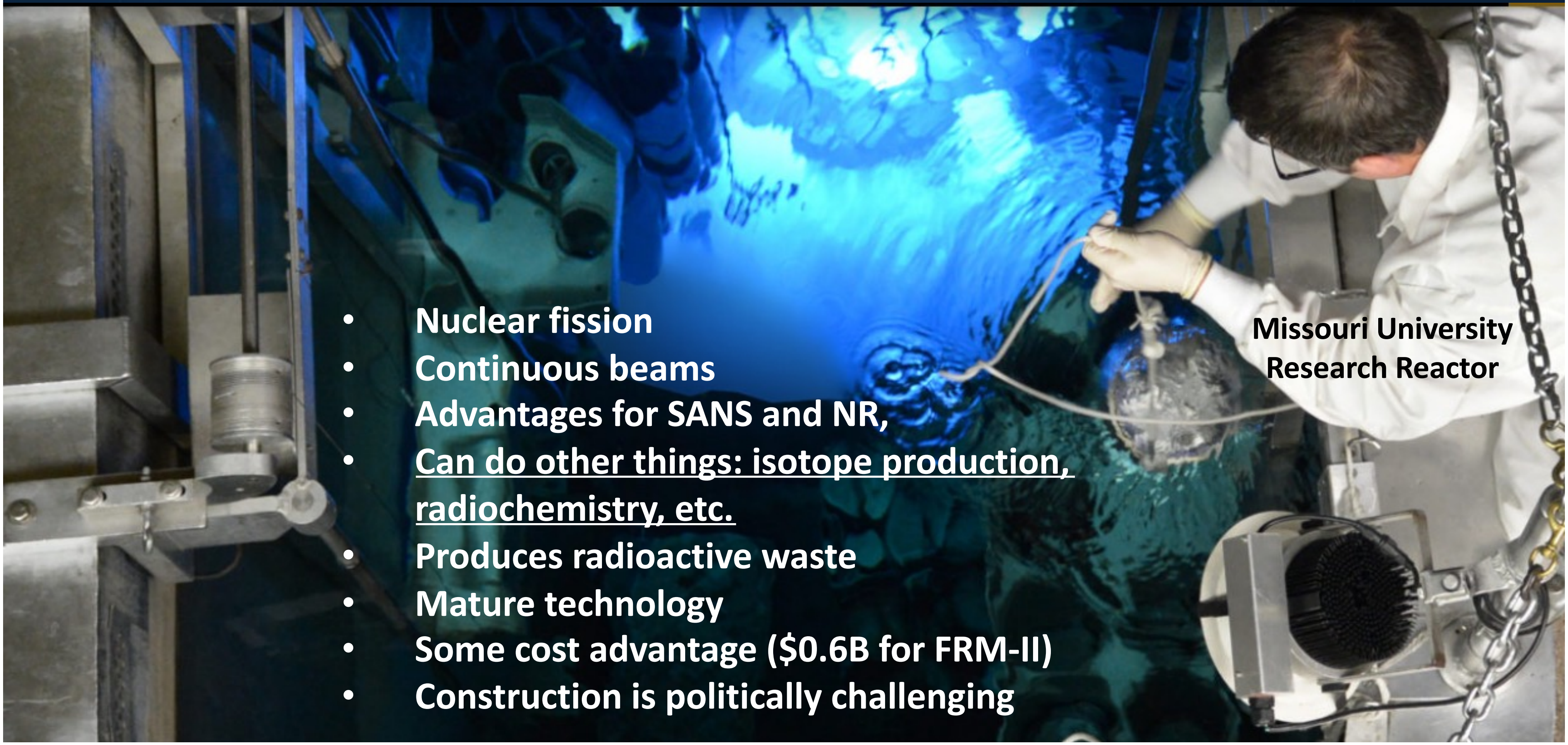
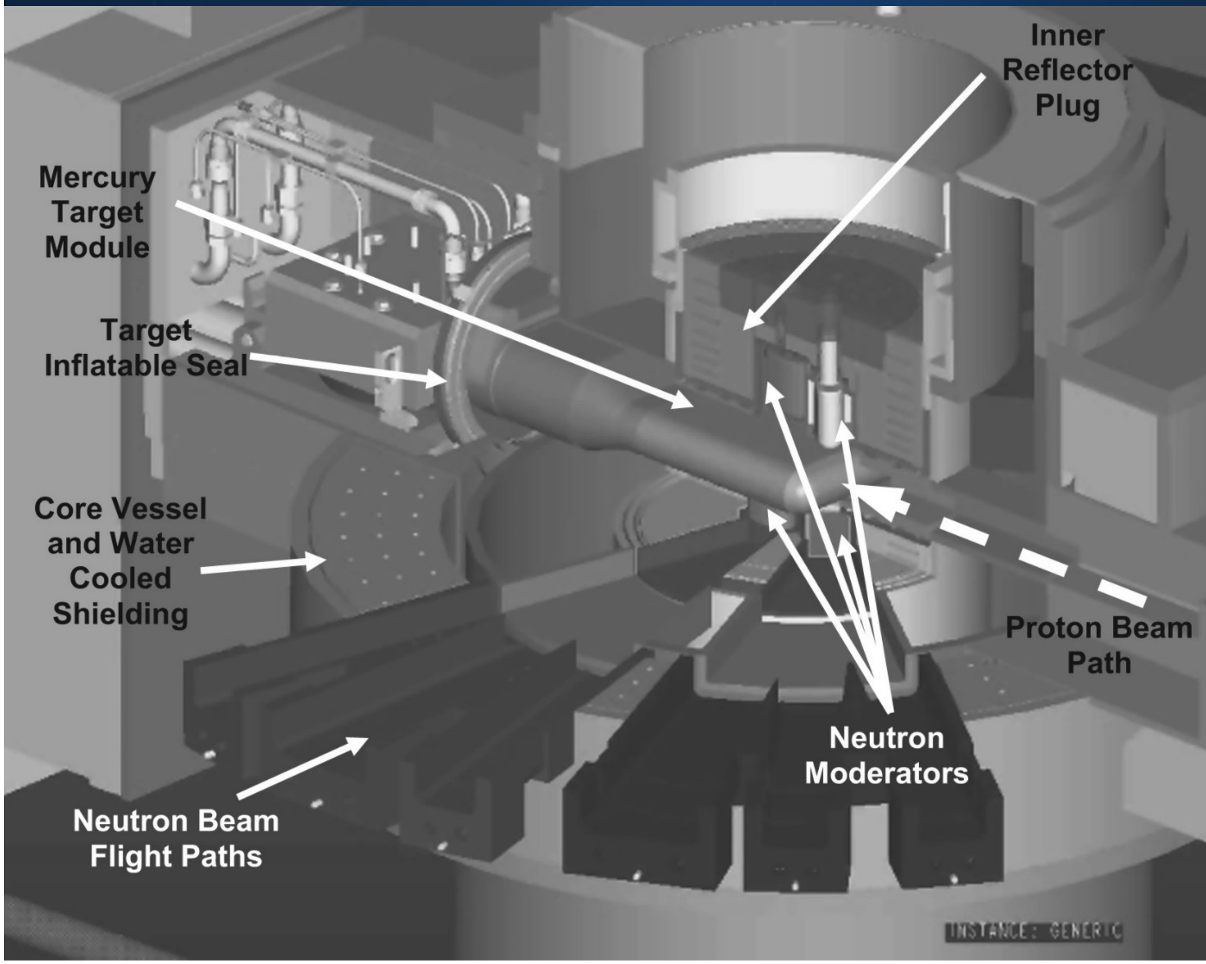


Missouri University Research Reactor

- Nuclear fission
- Continuous beams
- Advantages for SANS and NR,
- Can do other things: isotope production, radiochemistry, etc.
- Produces radioactive waste
- Mature technology
- Some cost advantage ($0.6B for FRM-II)
- Construction is politically challenging

Spallation Sources



- Accelerators crash protons into a heavy metal target
- Generally pulsed
- Advantages for crystallography, spectroscopy
- Not good for isotope production, radiochemistry, etc.
- <u>Limited radioactive waste</u>
- Complex, novel technology
- Large, expensive facilities ($2B for ESS, without instruments)

Mercury target at SNS

J. R. Haines et al., 10.1016/j.nima.2014.03.068

Sources

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FACILITY	LOCATION	TYPE	STARTUP
Institut Laue-Langevin (ILL)	France	58.3 MW Reactor	1972
ISIS Neutron & Muon Source	England	0.2 MW Spallation	1985
Research Neutron Source Heinz Maier-Leibnitz (FRM II)	Germany	20 MW Reactor	2004
Swiss Spallation Neutron Source (SINQ)	Switzerland	1 MW Spallation	1996
Japan Spallation Neutron Source (JSNS)	Japan	1 MW Spallation	2006
OPAL Multi-Purpose Reactor	Australia	20 MW Reactor	2006
High Flux Isotope Reactor (HFIR)	United States	85 MW Reactor	1966
Spallation Neutron Source	United States	1.4 MW Spallation	2006
NIST Center for Neutron Research (NCNR)	United States	20 MW Reactor	1969

- **Sources with state-of-the-art neutron scattering**
- **Capabilities are very roughly comparable**
- **All oversubscribed by factors of 2-3**

Challenge

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- **Neutrons are weakly interacting probes**
- **We can't make that many of them**
- **Only a few highly oversubscribed places to perform measurements (and they're getting old)**

For users lucky enough to perform an experiment, quality is frequently compromised by available time

Instrumentation & Optics

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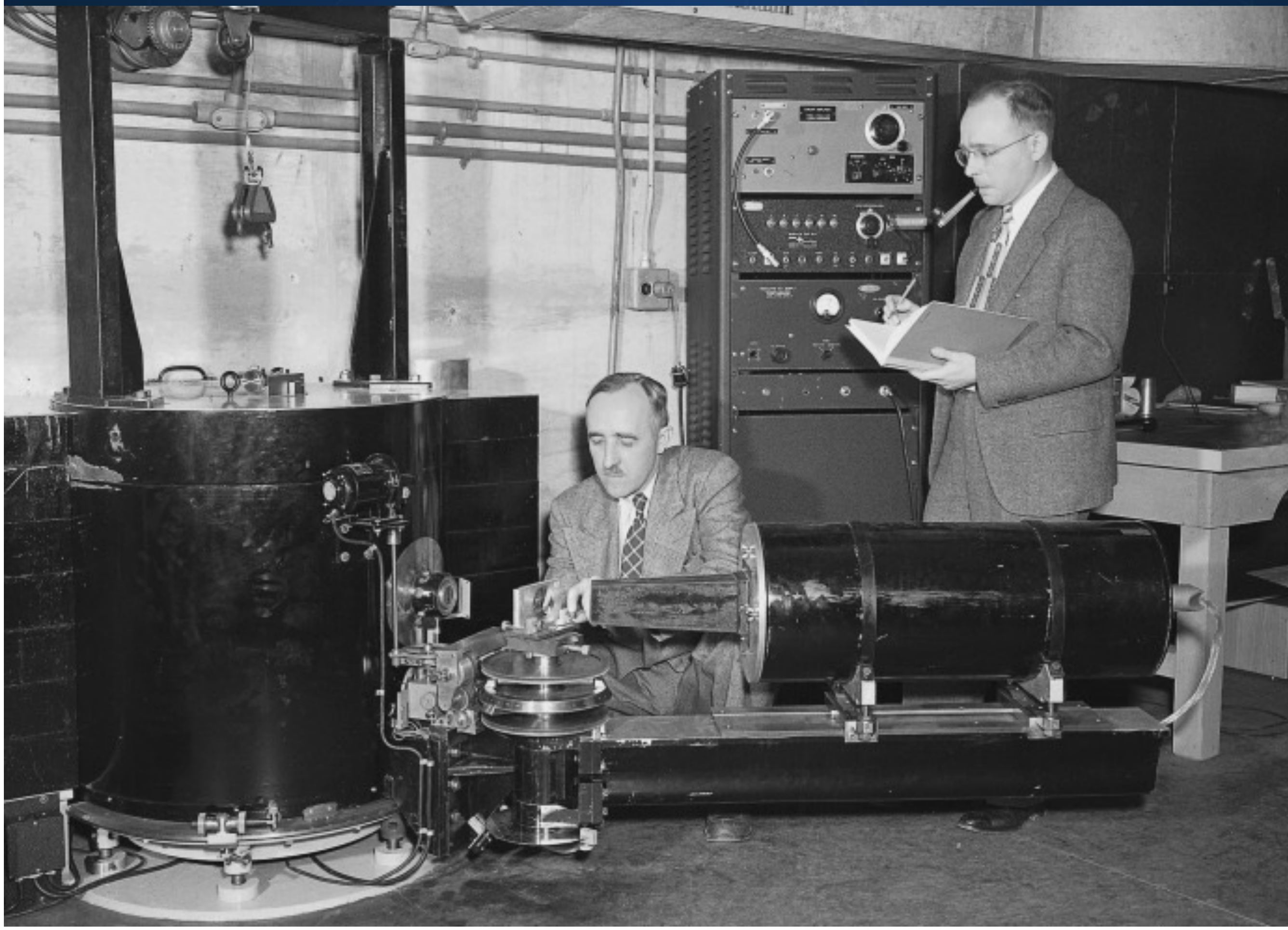

Source flux hasn't changed much in the past 50 years

Ernest Wollan and Cliff Shull, ORNL (actually more like 70 years ago)

Instrumentation & Optics

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Data rates have improved by 4 orders of magnitude in that time

CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NIST

Instrumentation & Optics

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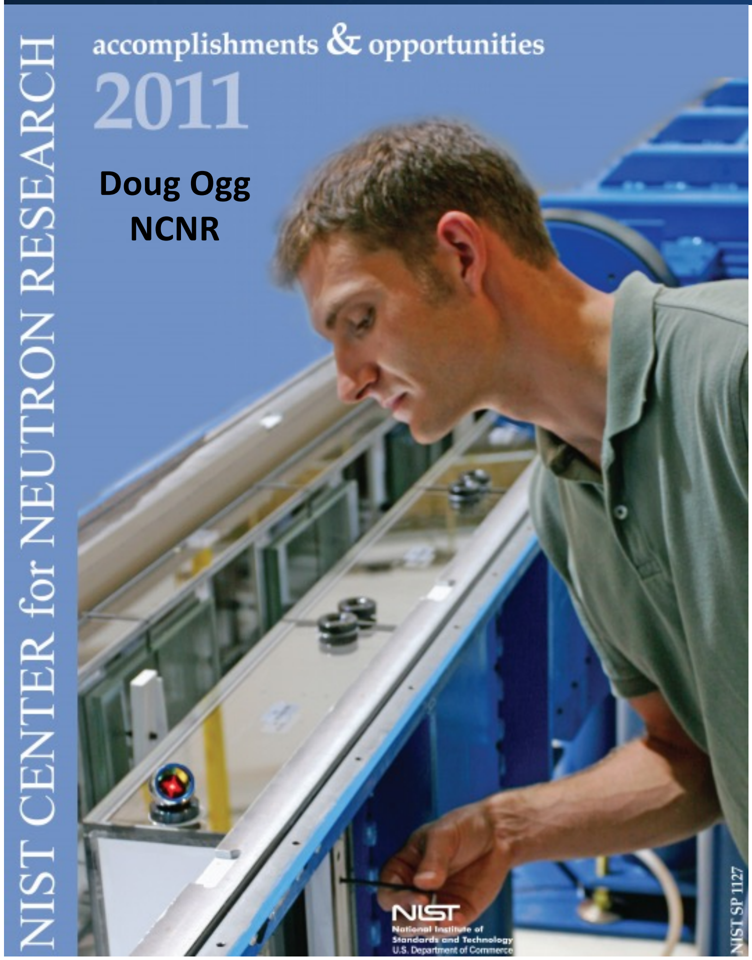
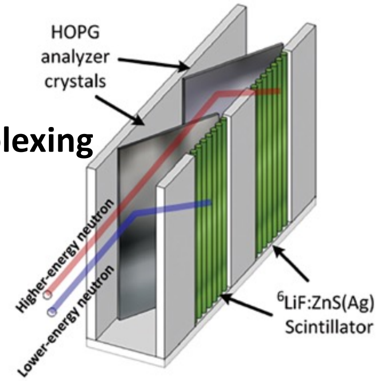


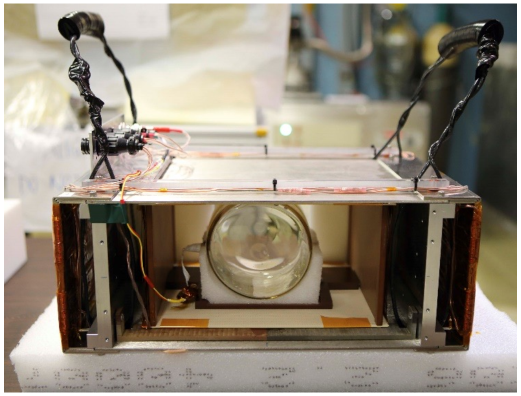
Doug Ogg
NCNR

- Optics (particularly guides)
- Detectors
- Beam Polarization
- Simulations

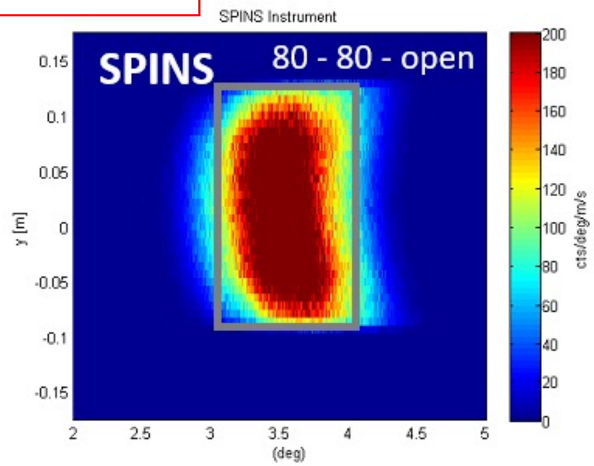
CANDOR multiplexing detector



Continue using technological advances for steady performance improvement



3He polarizing cell



Monte Carlo Sim

NCNR Moderator & Guide Upgrade

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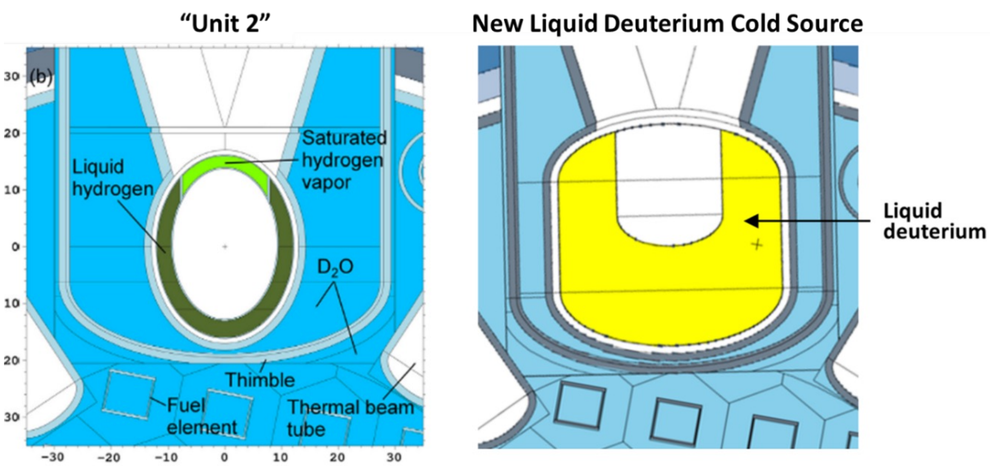
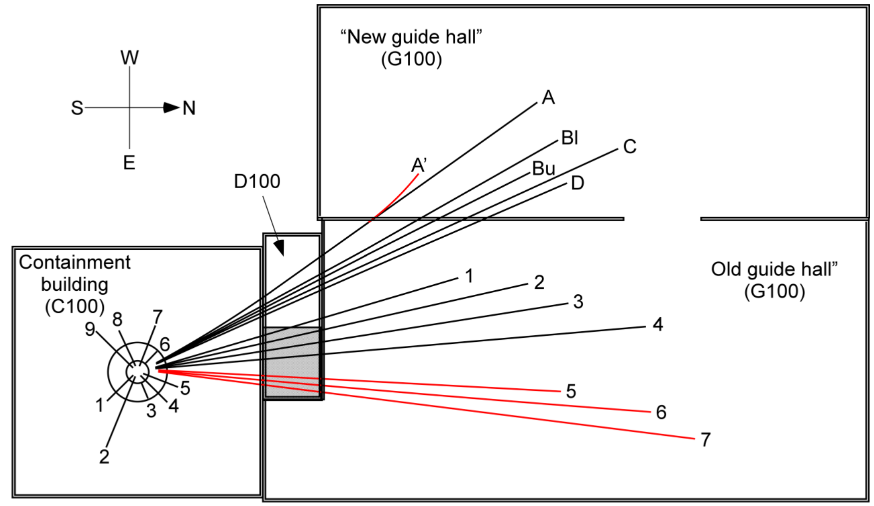
D_2 COLD SOURCE



NEW NG 5, 6, & 7

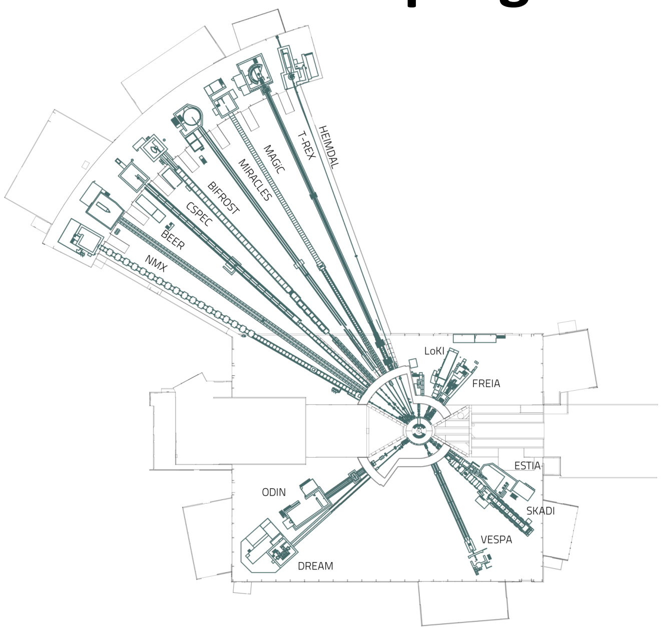


- D2 cold source ~2x gain for cold instruments
- New guides ~ 2x-4x data rate for many existing instruments
- New high performance instruments
- More capacity & new capabilities

European Spallation Source

NIST CENTER FOR NEUTRON RESEARCH

- Lund, Sweden
- Long-pulse
- World-leading intensity
- 2027 for user program



Oak Ridge Second Target Station

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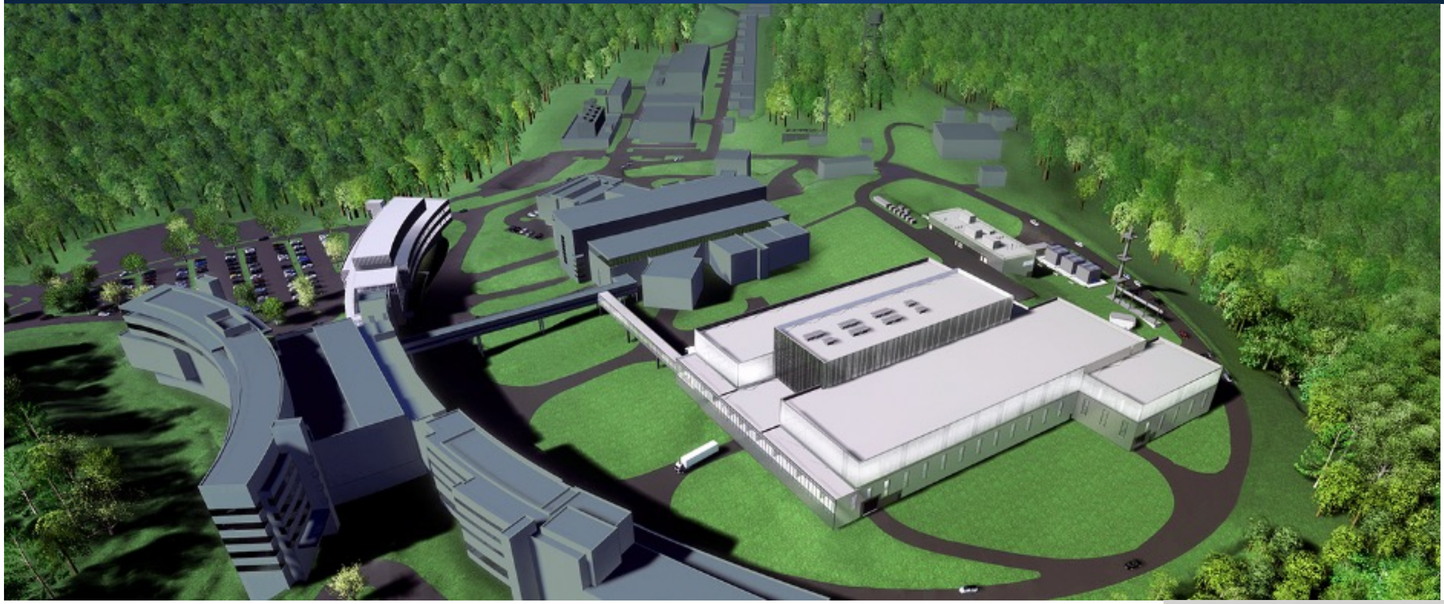
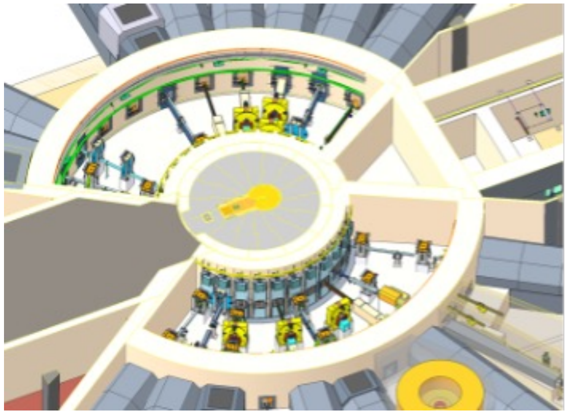
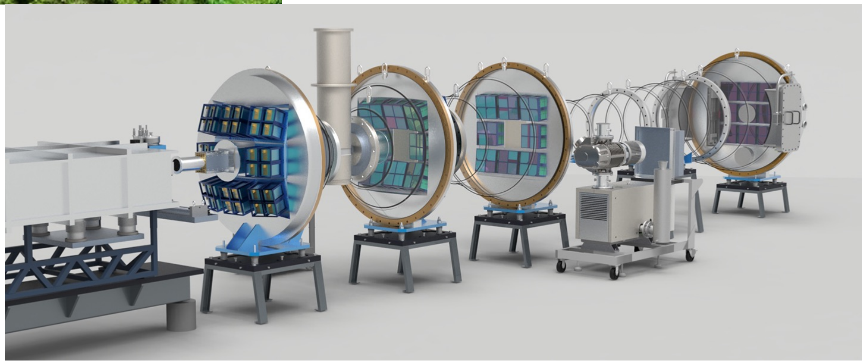




- **Optimized for cold neutrons**
- **World-leading peak brightness**
- **Timeline: late 2030s**



NIST New Neutron Source

CENTER FOR NEUTRON RESEARCH

- **<u>Pre-conceptual</u>** design work ongoing
- 20 MW, LEU, 2 cold sources, 2 GH
- CHiPS and Science Act requires NIST to produce a report for Congress that provides a strategic plan for the future of the NCNR
- "Neutrons for the Future" October 18-20, Rockville, MD

Proposed NIST Neutron Source User Facility

Jeremy C. Cook*, Hubert E. King*, Charles F. Majkrzak*, Dagistan Sahin*, Joy S. Shen*[†], Osman S. Celikten*, David Diamond*, Robert E. Williams*, Thomas H. Newton*

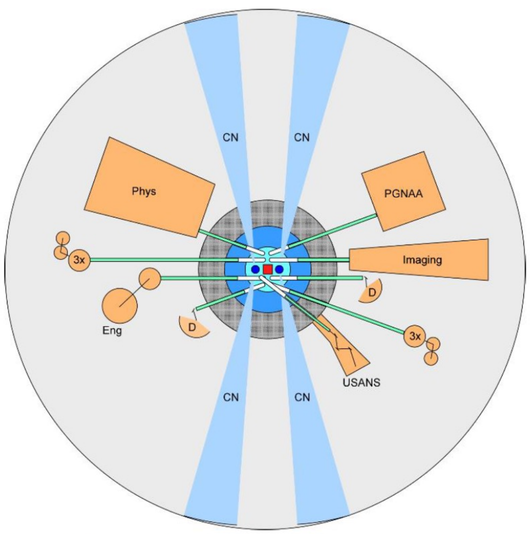


Figure 3: Beam guide configuration and thermal instruments.

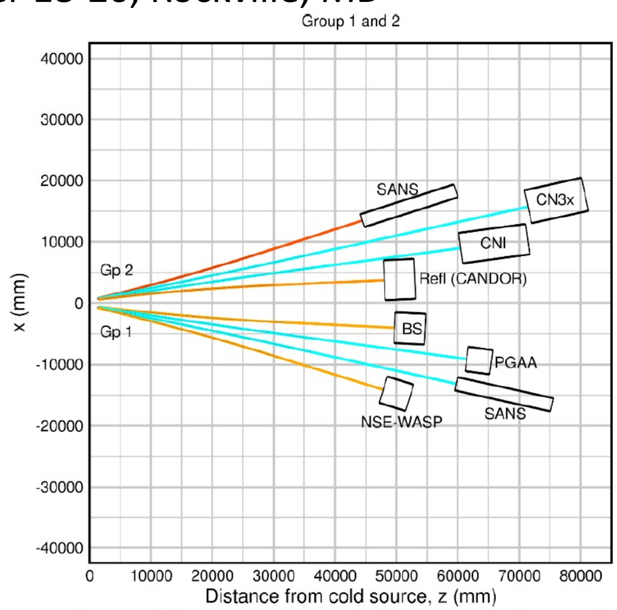


Figure 1. Possible Instrument Layout for Groups 1 and 2 (from Ref. [3]).

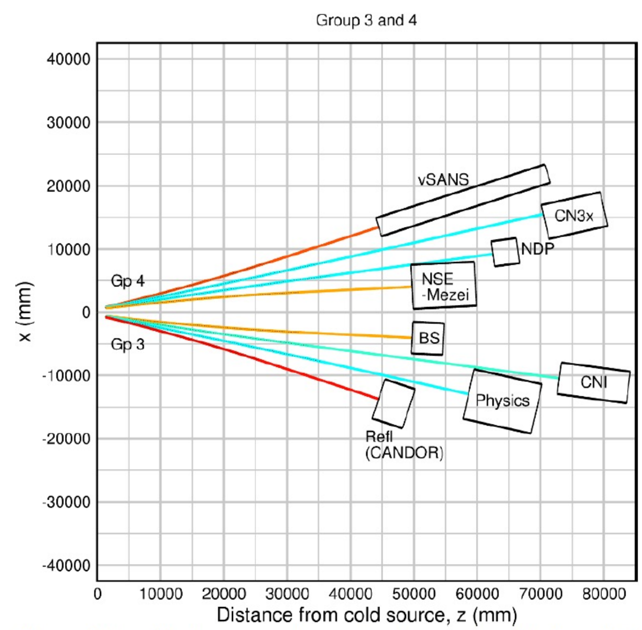


Figure 2 Possible Instrument Layout for Groups 3 and 4 (from Ref. [3]).

Neutrons as a National Resource

NIST CENTER FOR NEUTRON RESEARCH

- Microscopic structure and dynamics
- Sees what other probes can’t
- Sensitivity to light elements
  - Soft matter, biology
- Sensitive to magnetic fields
  - Quantum materials
- Weakly interacting
  - Highly penetrating
  - Exotic sample environments
- You have access – come see us