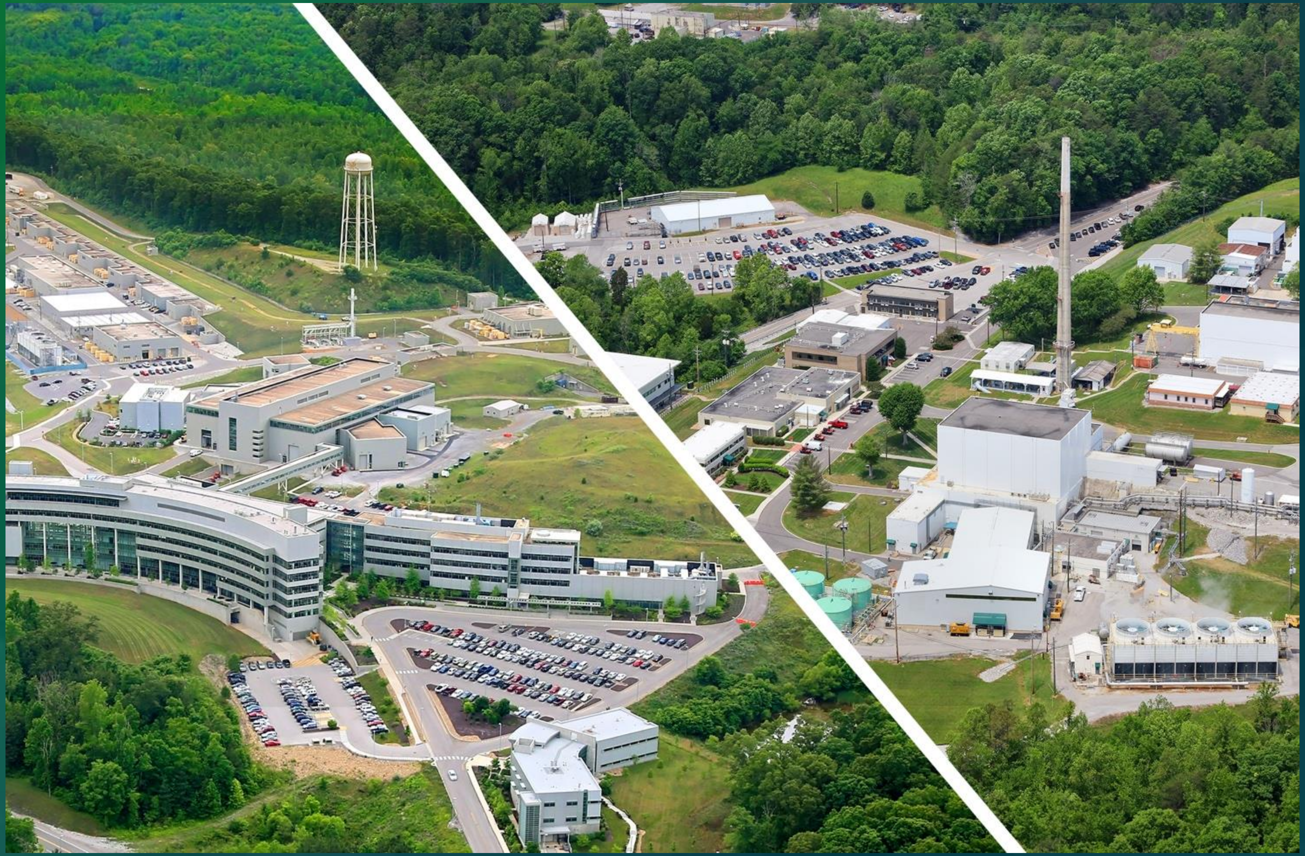
Neutron User Facilities

1st National Neutron Scattering School

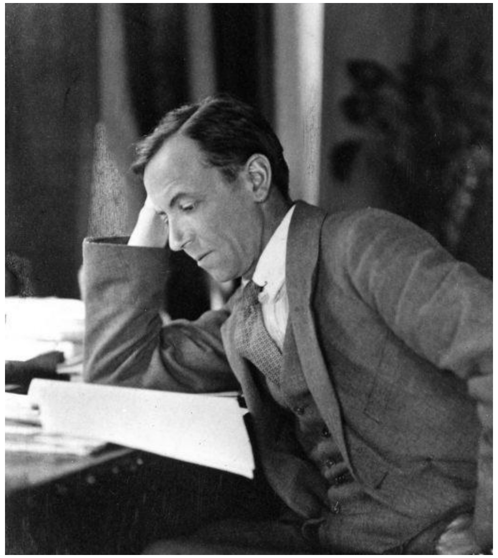


Mark Lumsden

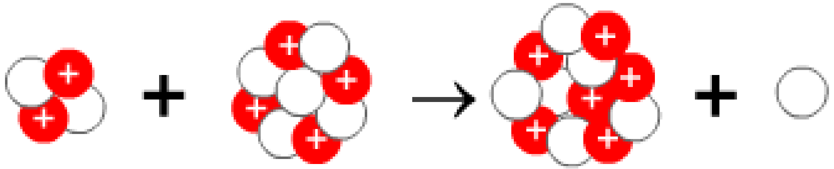
September 6th, 2025

The first neutron source

1935 Nobel Prize in Physics for the discovery of the neutron in 1932

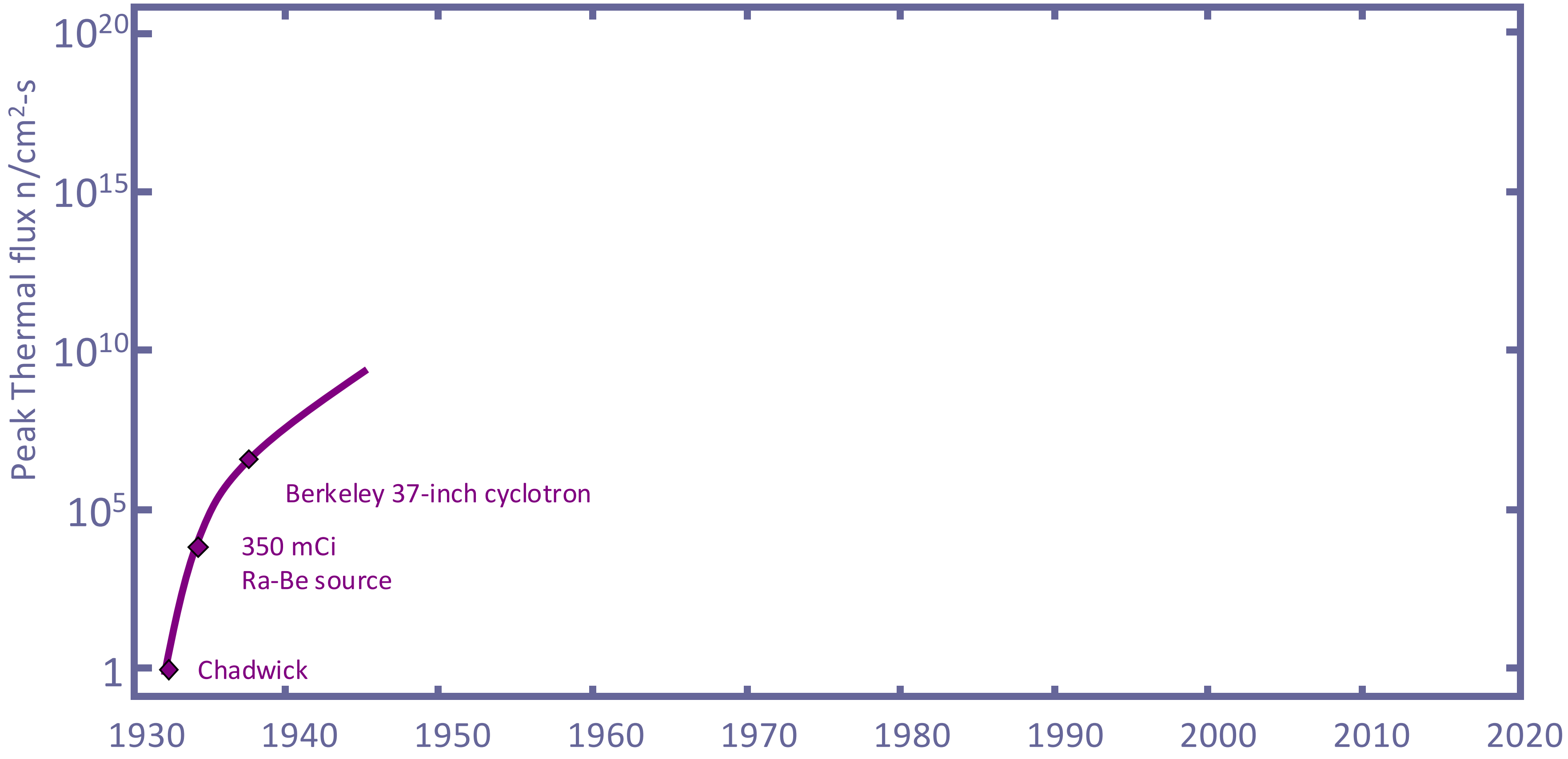


James Chadwick:
used Polonium as alpha emitter on Beryllium



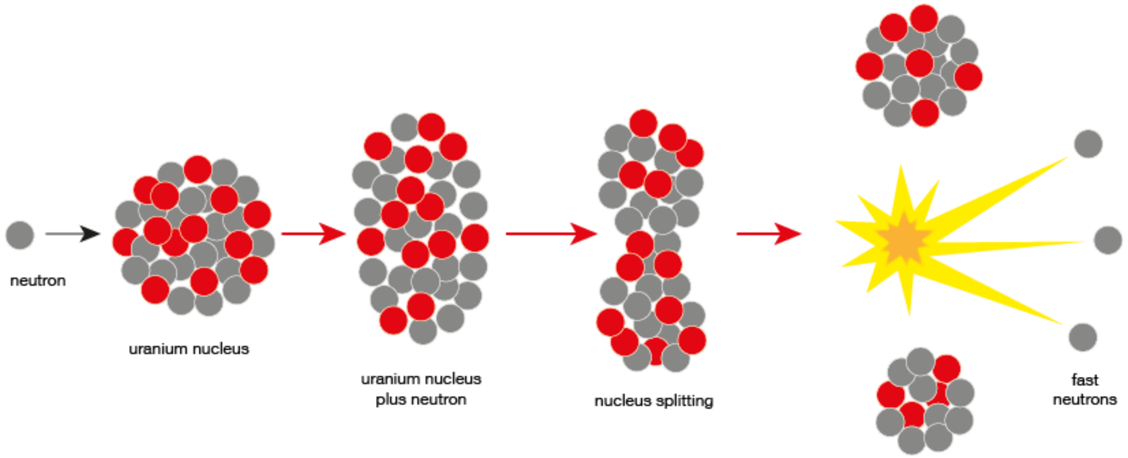
$$^{4}He + {}^{9}Be \rightarrow {}^{12}C + \text{neutron}$$

Evolution of neutron sources



(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

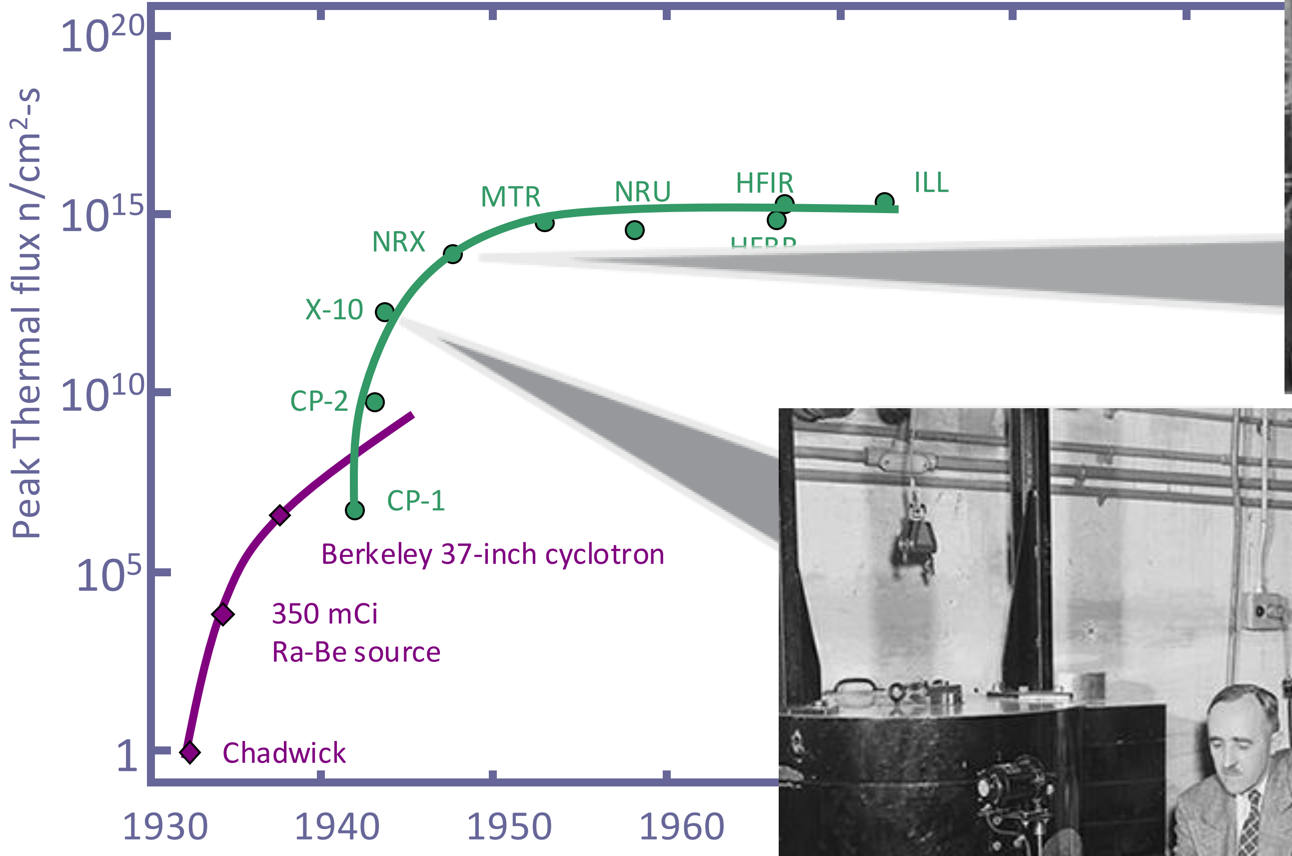
Nuclear fission



200 MeV/fission
2.35 – 1 = 1.35 excess neutrons
$\Rightarrow$ 150 MeV/neutron

December 2, 1942

Evolution of neutron sources

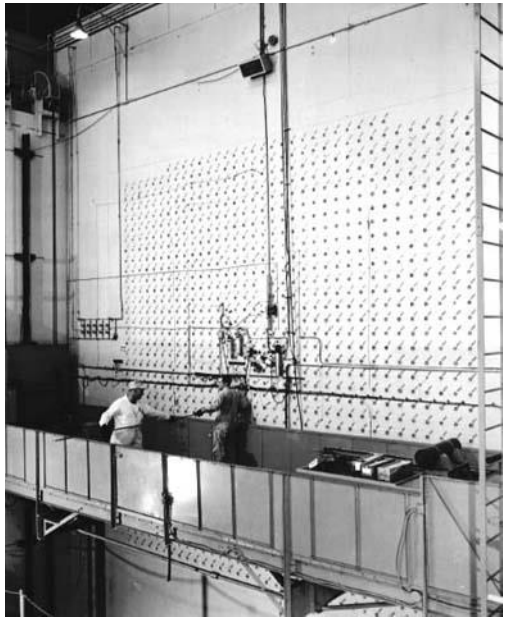


(Updated from *Neutron Scattering*, K. Sköld

1994 Nobel Prize in Physics:
"for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

Nuclear Reactor Power Drives Scientific Innovation

ORNL Graphite reactor
Critical on **Nov. 4, 1943**



Maximum power ~4 MW

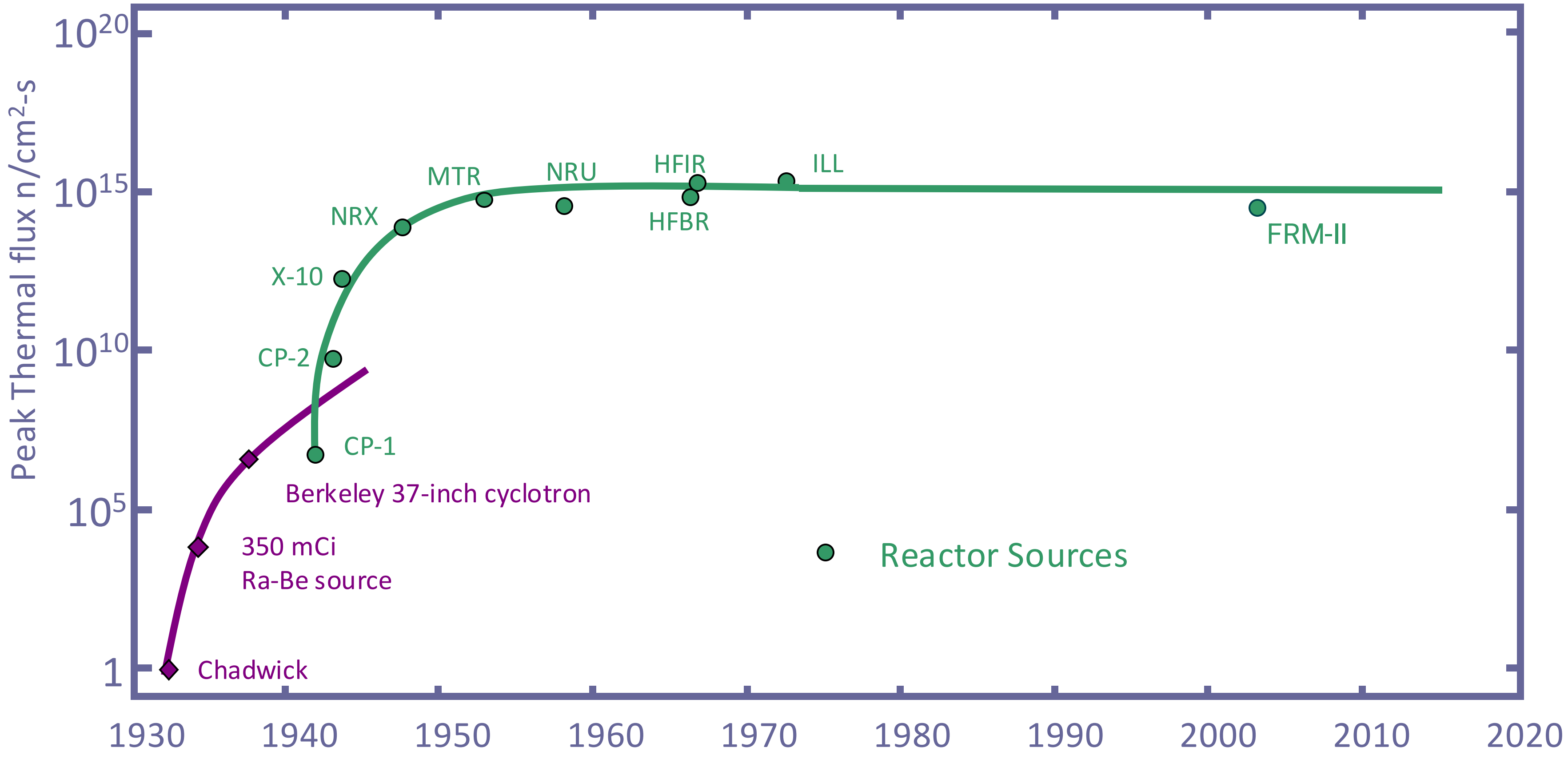
Chalk River NRX Reactor
Critical on **July 22, 1947**

- maximum power 42 MW
- **100-200 times more neutrons than Graphite Reactor!**

Chalk River NRU Reactor
Critical on **Nov. 3, 1957**

- Original design 200 MW with natural uranium
- Changed to 60 MW with high enriched Uranium
- Changed to 135 MW with low enriched Uranium

Evolution of neutron sources



(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

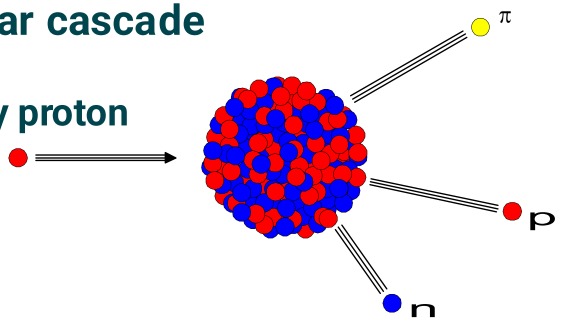
OAK RIDGE
National Laboratory

Nuclear spallation

1 GeV proton in:
250 MeV becomes mass (endothermic reaction)
30 neutrons freed
⇒ 25 MeV/neutron
6x more efficient than fission

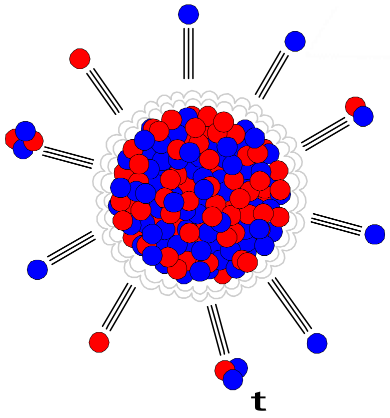
First stage: intranuclear cascade

high-energy proton

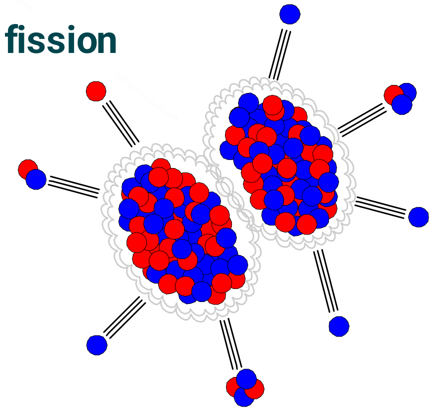


Intermediate stage: pre-equilibrium

evaporation

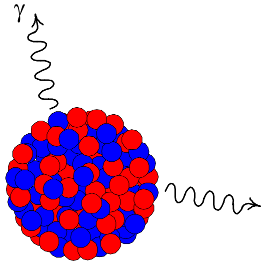


fission

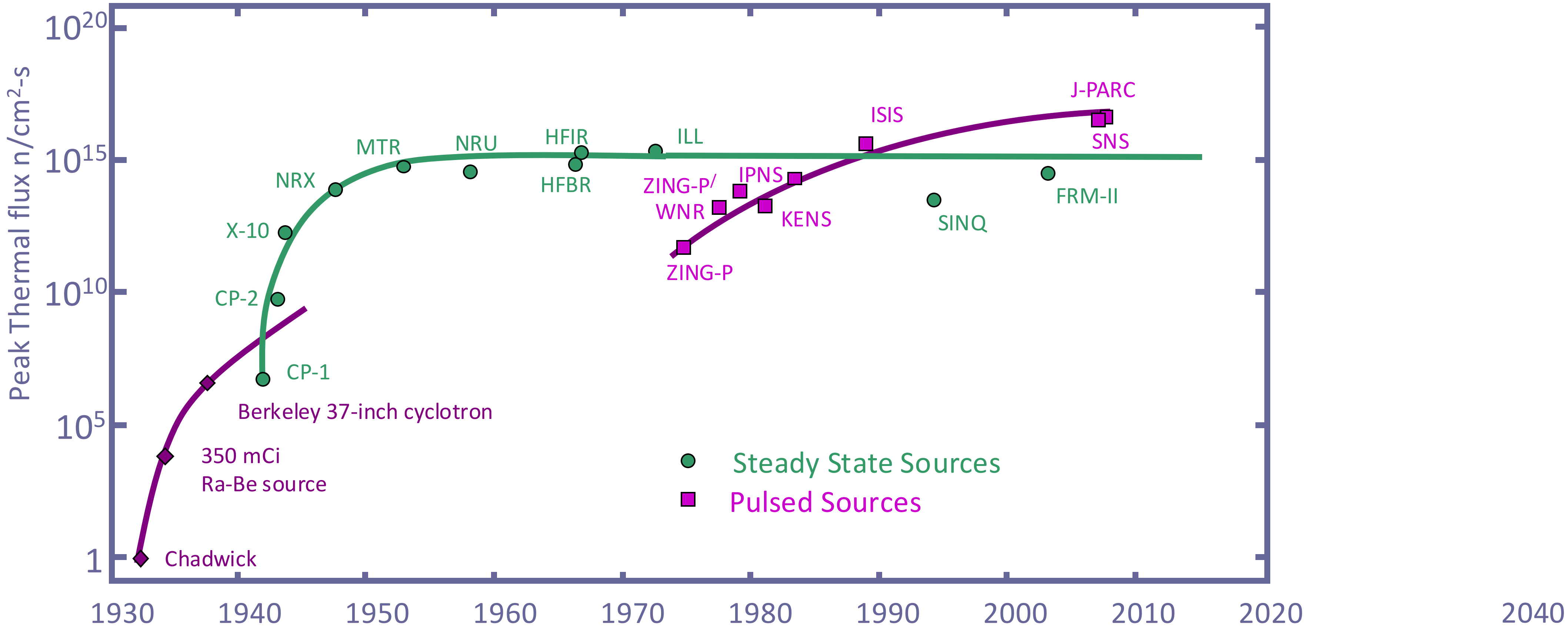


Reminder – fission:
200 MeV/fission
2.35 – 1 = 1.35 excess neutrons
⇒ 150 MeV/neutron

Final stage: residual de-excitation



Evolution of neutron sources



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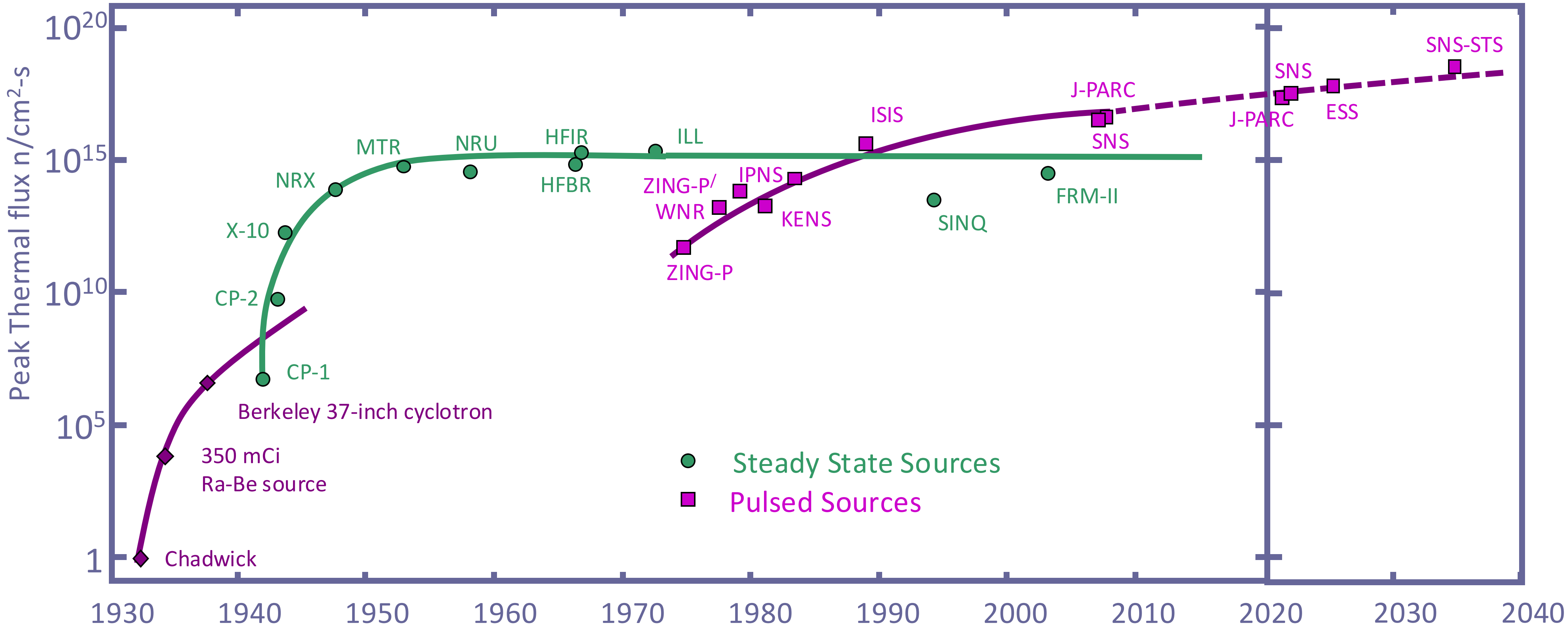
Evolution of neutron sources



(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

OAK RIDGE National Laboratory

Institut Laue-Langevin (France): The First User Facility

- ILL founded 1967
  - First experiments 1972
  - International: France, Germany, UK
- A "Service Institute"
  - Accessible to non-experts
  - Support from an expert "local contact"
  - Support for travel
  - Access based on scientific merit
  - Peer review of proposals
  - Twice-yearly proposal rounds

- Until then, large-scale facilities were mainly for in-house expert users and their collaborators

User Facilities

- Neutrons invented user facilities
  - Importance of technique
  - High cost
  - Small science
- Now a widespread business model in science
- Department of Energy Office of Science definition:
  - Open to all without regard to nationality or affiliation
  - Access based on merit review
  - Free to use if results are to be published
  - Facility allows safe and efficient work
  - Facility supports user organization to represent users and promote collaboration
  - Facility does not compete with private sector capability

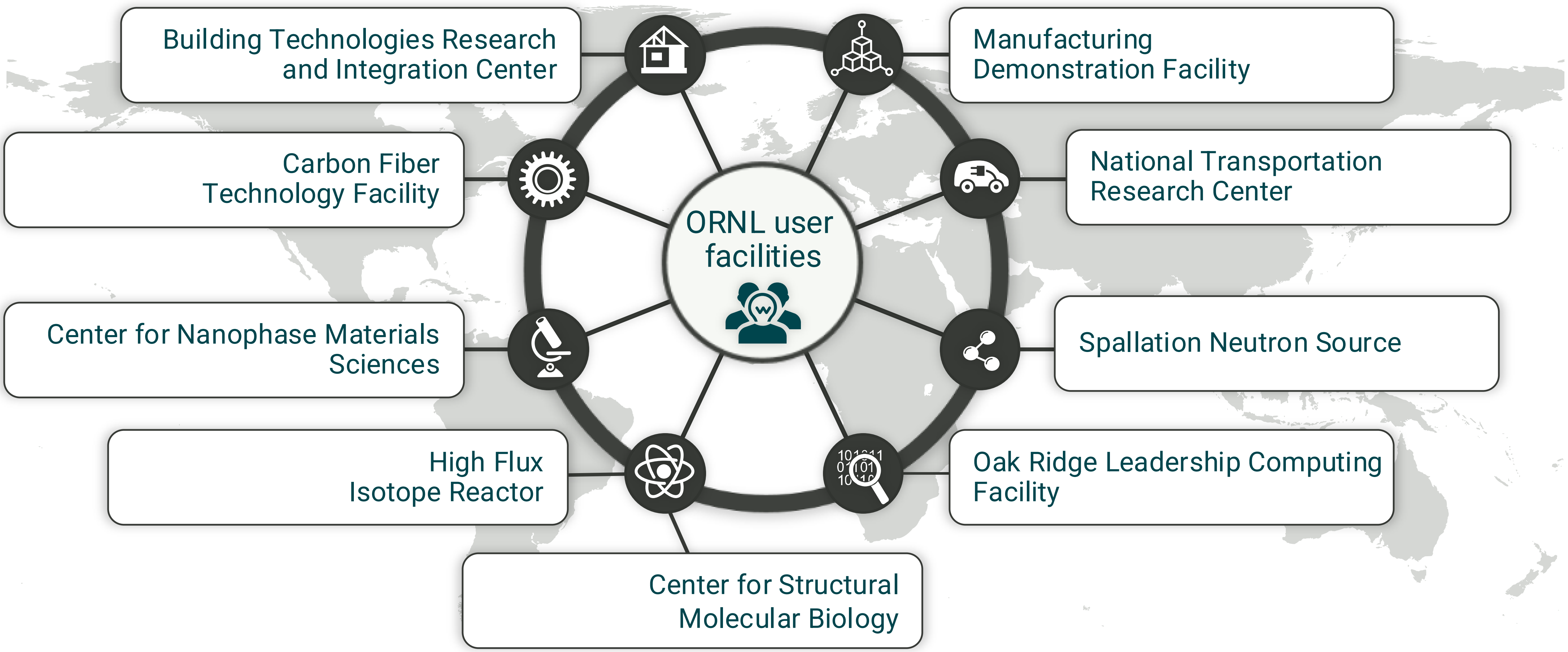
Office of Science User Facilities List:

- Fermi accelerator complex (FermiLab)
- **Argonne Leadership Computing Facility (ANL)**
- **Advanced Light Source (LBNL)**
- **Advanced Photon Source (ANL)**
- Atmospheric Radiation Measurement user facility
- Accelerator Test Facility (BNL)
- Argonne Tandem Linac Accelerator System (ANL)
- Continuous Electron Beam Accelerator Facility (TJNAF)
- **Center for Functional Nanomaterials (BNL)**
- **Center for Integrated Nanotechnologies (LANL / SNL)**
- **Center for Nanoscale Materials (ANL)**
- **Center for Nanophase Materials Sciences (ORNL)**
- DIII-D National Fusion Facility (GA)
- Environmental Molecular Sciences Laboratory (PNNL)
- **Energy Sciences Network (LBNL)**
- Facility for Advanced Accelerator Experimental Tests (SLAC)
- Facility for Rare Isotope Beams (Michigan State)
- **High Flux Isotope Reactor (ORNL)**
- **National Synchrotron Light Source II (BNL)**
- Joint Genome Institute (LBNL)
- **Linac Coherent Light Source (SLAC)**
- **National Energy Research Scientific Computing Center (LBNL)**
- National Spherical Torus Experiment (Princeton)
- **Oak Ridge Leadership Computing Facility (ORNL)**
- Relativistic Heavy Ion Collider (BNL)
- **Spallation Neutron Source (ORNL)**
- **Stanford Synchrotron Radiation Light Source (SLAC)**
- **The Molecular Foundry (LBNL)**

- **Neutron Sources**
- **Light Sources**
- **Nanoscience Centers**
- **Computing**

28 Office of Science User Facilities

Oak Ridge National Laboratory User Facilities



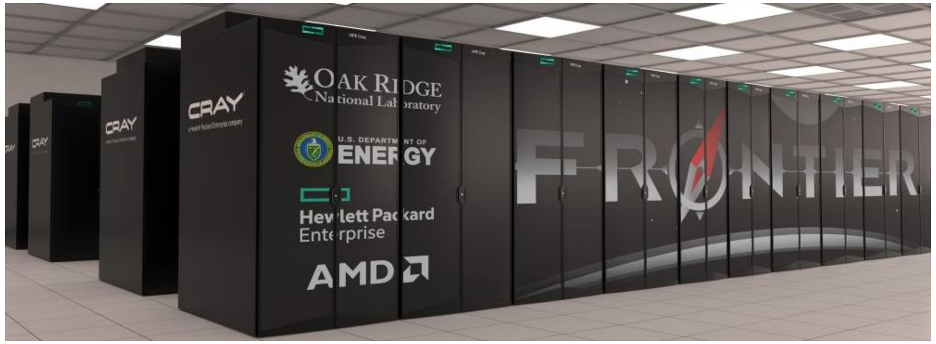
OAK RIDGE National Laboratory

Oak Ridge Leadership Computing Facility (OLCF)

- Computing and Computational Sciences Directorate (CCSD) houses the Oak Ridge Leadership Computing Facility, home to ***Frontier***
- Provides expertise in data science, modeling and simulation for grand challenge science. Advances the state-of-the-art in artificial intelligence, data science and quantum information science
- Researchers can apply for time at leadership computing facilities through several allocation programs that cater to a range of scientific disciplines and HPC experience levels
- Since 2006, the Oak Ridge Leadership Computing Facility has deployed four supercomputers that debuted as fastest in the world, including Summit in 2018 and Frontier in 2022 - the ***first exascale machine in the world***.

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

DOE Exascale Computing Initiative (2016-2024) produced three systems exceeding an ExaFlop/s performance



Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
4	**JUPITER Booster** - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN EuroHPC/FZJ Germany	4,801,344	793.40	930.00	13,088
5	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	
6	**HPC6** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, RHEL 8.9, HPE Eni S.p.A. Italy	3,143,520	477.90	606.97	8,461

Frontier is the fastest supercomputer for open science

Center for Nanophase Materials Sciences

A user facility for nanoscale and quantum materials

- **Broad spectrum of imaging capabilities**
  - scanning transmission electron microscopy (now down to 4.5 K) emphasizing electron energy loss spectroscopy
  - scanning probe microscopies He-ion microscopy
  - atom probe tomography
  - mass spectrometry-based chemical imaging

- The Center for Nanophase Materials Sciences (CNMS) at ORNL offers the user community access to state-of-the-art equipment for a broad range of nanoscience research, including nanomaterials synthesis, nanofabrication, imaging/ microscopy/characterization, and theory/modeling/simulation.
- Access is obtained through a peer-reviewed proposal with no charge for users who intend to publish their results in the open literature.
- CNMS also acts as gateway for the nanoscience community to benefit from ORNL's neutron sources (**SNS and HFIR**) and computational resources.

Center for Structural Molecular Biology

Deuteration access through SNS/HFIR User Program

- **Biological H/D labeling** of cells, proteins, nucleic acids, lipids, uniform, selective labeling
- **Biomolecule purification** and characterization
- **Chemical deuteration** in collaboration with the CNMS
- **Supporting capabilities**: protein crystallography, SAXS

- The Center for Structural Molecular Biology (CSMB) at ORNL is an open access user program dedicated to advancing instrumentation and methods for determining the three-dimensional structures of biomacromolecules and their assemblies as well as hierarchical structures and biomimetic systems.

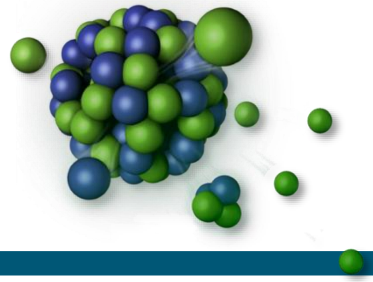
- The centerpiece of the CSMB is a SANS instrument at HFIR dedicated to studying biological samples (Bio-SANS).

- CSMB also operates a Bio-Deuteration Laboratory for cloning, protein expression, purification, and characterization of H/D-labeled biological macromolecules. When deuterium labeling is combined with SANS experimentation, data analysis and visualization, models of complex systems can be constructed that are not obtainable using other techniques.

ORNL operates two advanced neutron scattering user facilities

High Flux Isotope Reactor (HFIR)

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



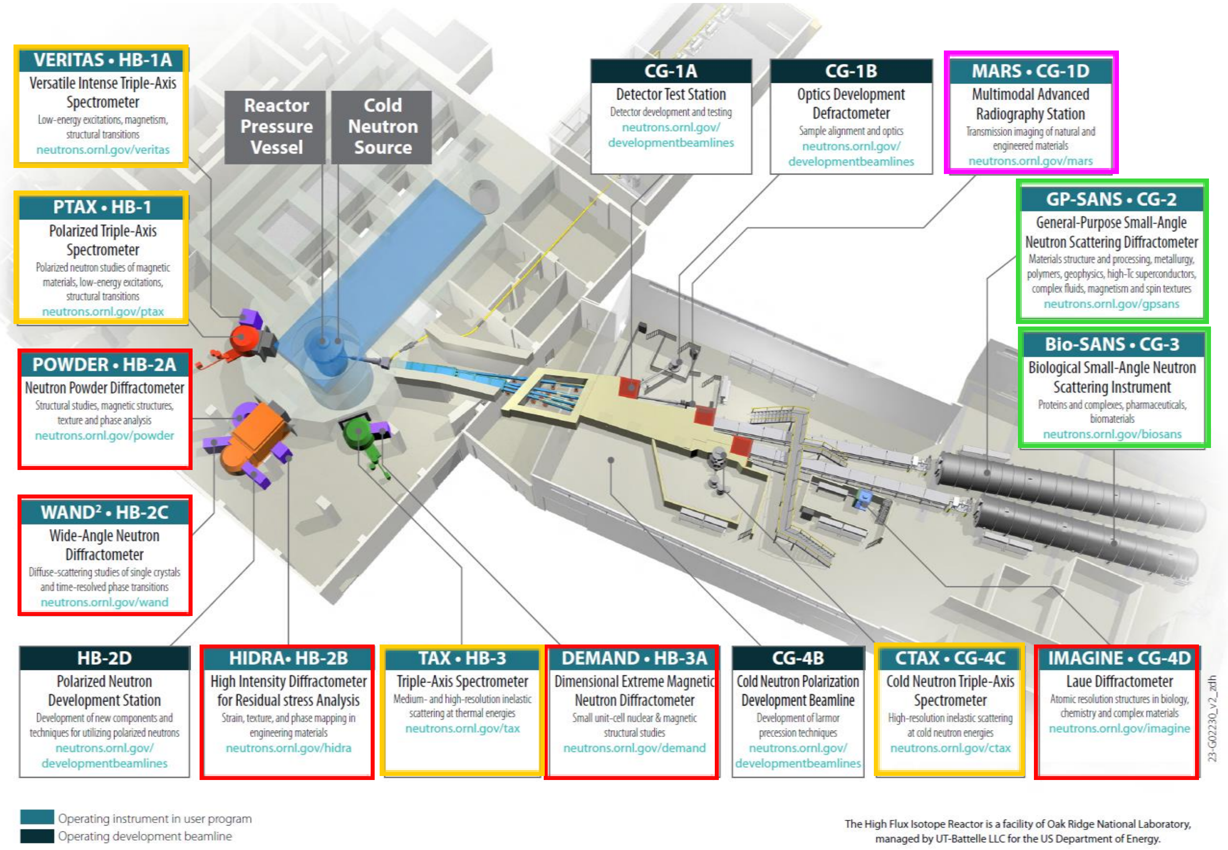
- **85 MW steady state neutron source.**
- **Peak thermal flux of 2.5 x 10^{15} neutrons/cm^2/s**
- **Neutron scattering, isotopes, materials irradiation**
- **Isotopes: Cf-252, Pu-238, Ac-227, Ni-63**
- **12 instruments for neutron scattering & imaging**

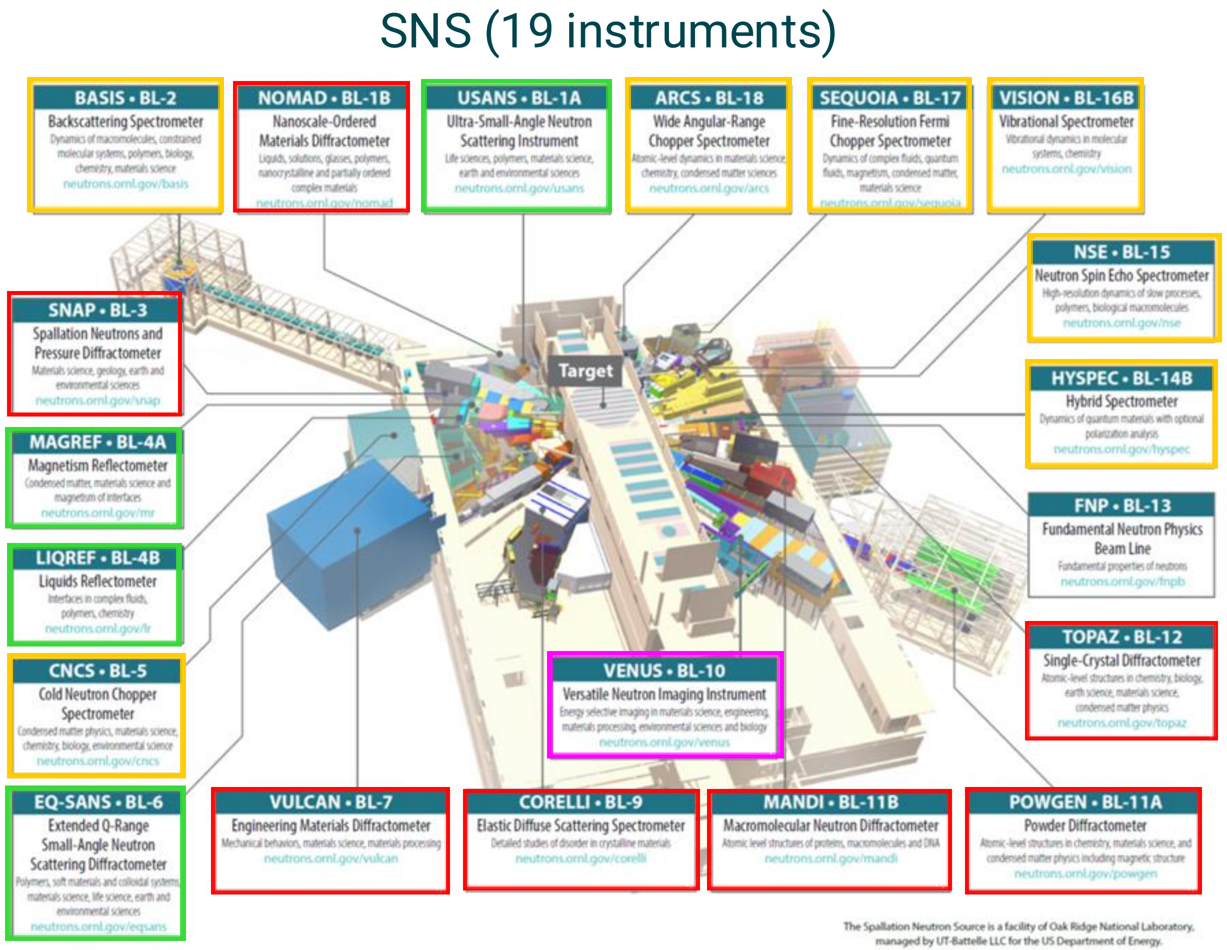
Spallation Neutron Source (SNS)

- **1.8 MW operating power (upgrading to 2 MW)**
- **Worlds highest power proton accelerator**
  - **1.3 GeV protons: 30 kJ/proton pulse**
- **60 Hz pulsed neutron source (695 ns pulse width)**
- **19 instruments for neutron scattering & imaging**

OAK RIDGE National Laboratory

Instruments at HFIR and SNS





Diffraction (elastic scattering) (12 instruments)

Spectroscopy (inelastic scattering) (11 instruments)

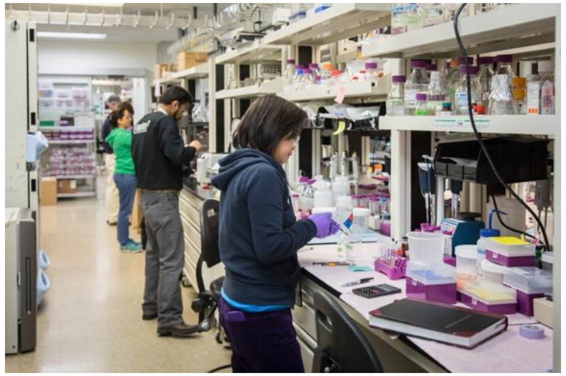
SANS & Reflectometry (elastic scattering) (6 instruments)

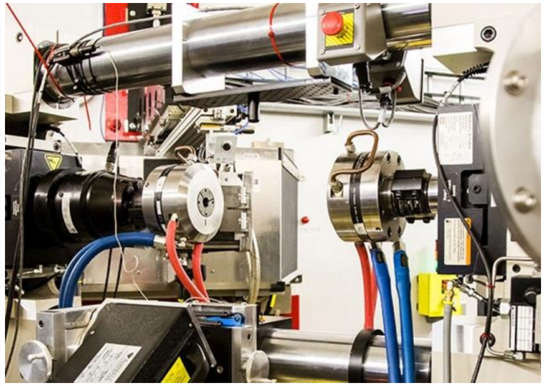
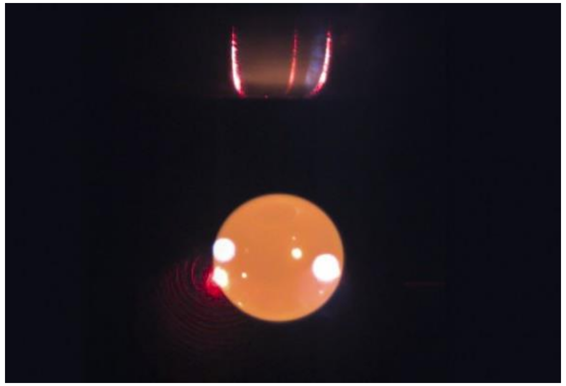
Neutron Imaging (2 instruments)

Oak Ridge National Laboratory

Sample Environment and Complementary Facilities





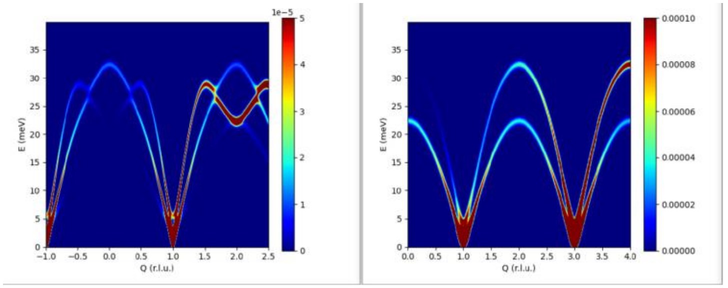
- Experiments are increasingly complex – few ‘routine’ measurements. This requires increasingly complex sample environments.
- Complementary laboratory facilities are needed for sample preparation (including deuteration) and characterization

Modeling and AI / ML to interpret neutron scattering data

INSPIRED: Inelastic Neutron Scattering Prediction for Instantaneous Results and Experimental Design

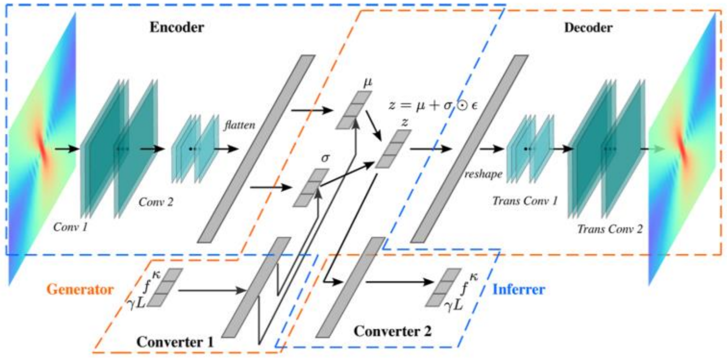
DFT + ***OCLIMAX*** - simulate lattice dynamics & make a database of simulated spectra (>10k inorganic crystals and >20k organic molecules).

Machine learning prediction of INS from structure



Bowen Han, Andrei T. Savici, Mingda Li, and Yongqiang Cheng, Comp. Phys. Commun. **304**, 109288 (2024)

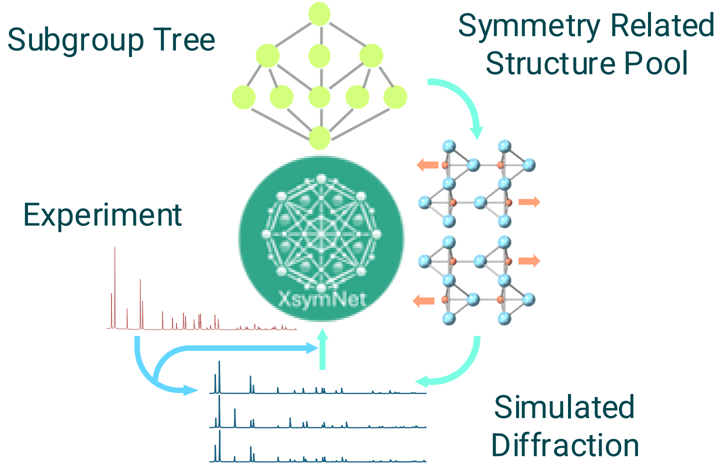
Machine Learning assisted SANS Data Analysis



Deep learning approach to analyzing 2D SANS data. Produces similar answers to conventional fitting but >1000 times faster.

Lijie Ding, Chi-Huan Tung, Bobby G. Sumpter, Wei-Ren Chen, and Changwoo Do, J. Chem. Theory Comput. **21**, 4176 (2025)

XsymNet: Combined Exhaustive Symmetry & Deep Learning Framework



A convolutional neural network with multihead attention, trained on an exhaustive listing of structures in the possible phase transition pathways.

Identifies the lattice, symmetry, and atomic distortions from powder diffraction data.

Dayton Kizzire, Powder Diffraction Group

Becoming a neutron scattering user at SNS or HFIR

- Prospective users should submit a proposal to one of our biannual proposal calls
- 2026-A GU proposal call for HFIR submissions only is open now and will close on Oct. 1, 2025.
- 1500+ General User proposals requesting beam time are received annually

- ***New users should contact an instrument scientist for feedback on their experimental plan before submitting***

- More information and tips on submitting a proposal can be found at https://neutrons.ornl.gov/users

Future: Upgrades to the SNS accelerator and the addition of the "Second Target Station" will provide next generation capabilities

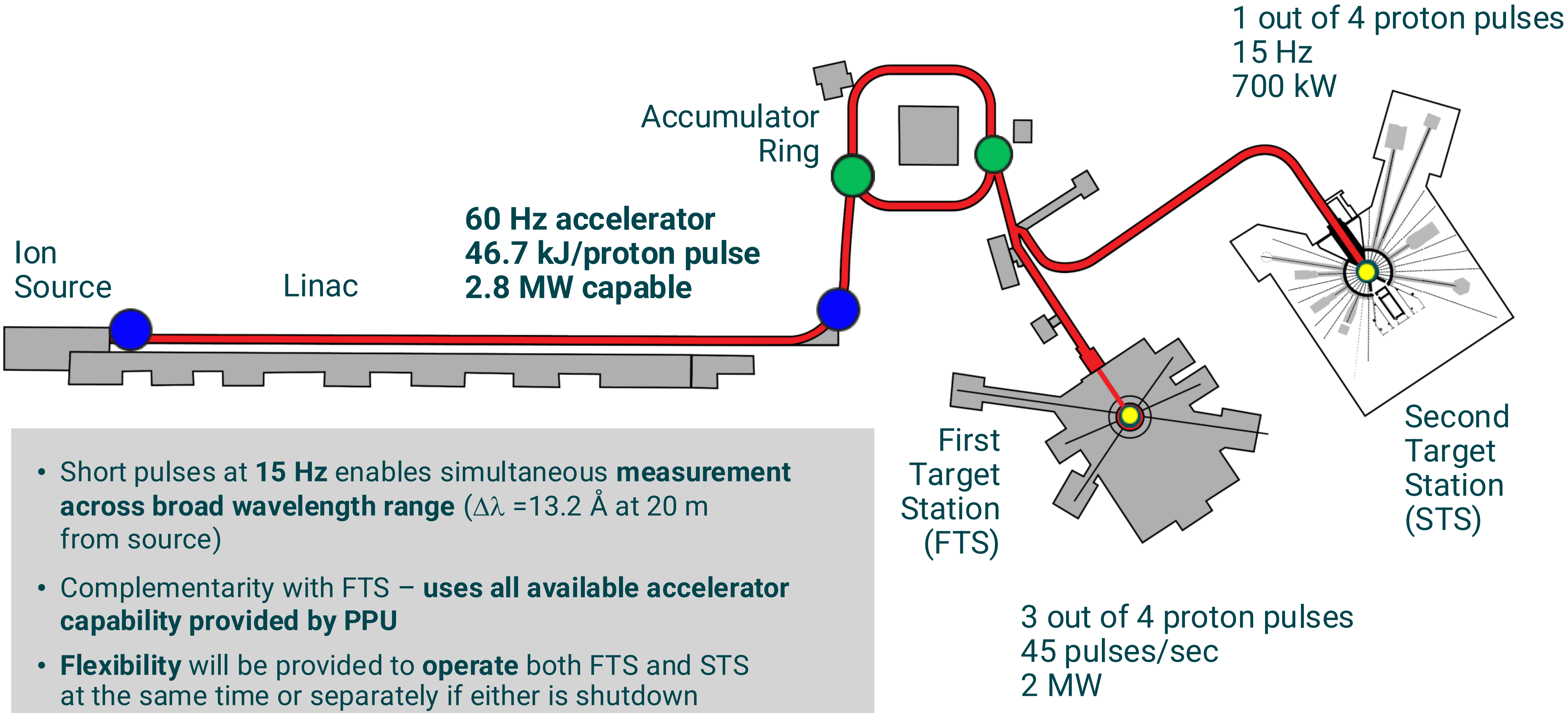
PPU project: Double the power of the existing accelerator structure

- First Target Station (FTS) is optimized for thermal neutrons
- Increases the brightness of beams of pulsed neutrons
- Provides new science capabilities for atomic resolution and fast dynamics
- Provides a platform for STS

STS project: Build the second target station with initial suite of beam lines

- Optimized for cold neutrons
- World-leading peak brightness
- Provide new science capabilities for measurements across broader ranges of temporal and length scales, real-time, and smaller samples

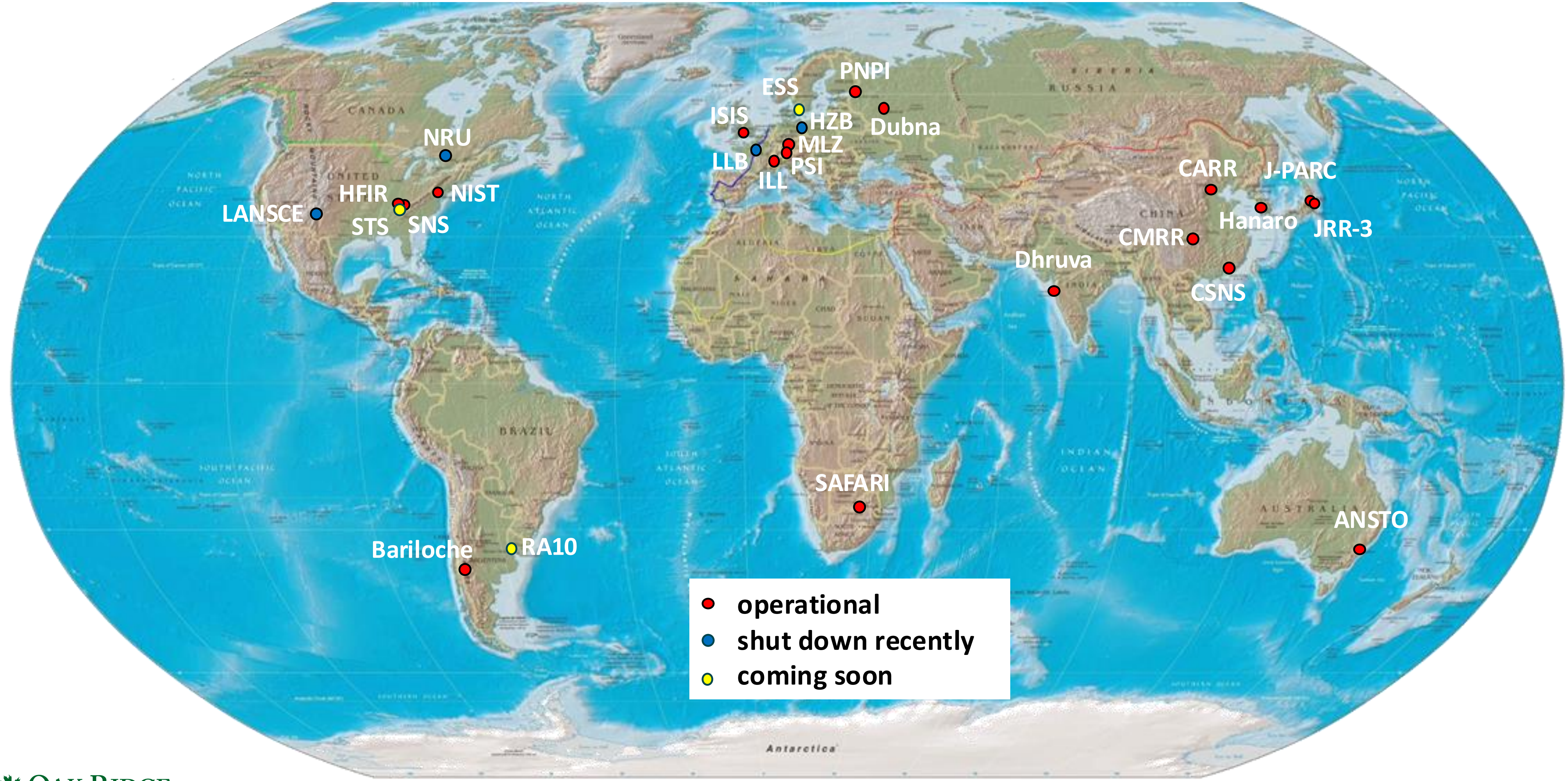
STS will make optimal use of the PPU-upgraded SNS accelerator capability



- Short pulses at **15 Hz** enables simultaneous **measurement across broad wavelength range** ($\Delta\lambda$ =13.2 Å at 20 m from source)
- Complementarity with FTS – **uses all available accelerator capability provided by PPU**
- **Flexibility** will be provided to **operate** both FTS and STS at the same time or separately if either is shutdown

*animation courtesy of Matt Stone

Neutron User Facilities Worldwide



Neutron Facility Ecosystem

2018

International "flagship" facilities: ILL, ISIS, SNS, J-PARC

regional/national	Europe	North America	Asia	Others
high-flux & medium-flux scattering facilities	MLZ, PSI, LLB, HZB	NIST, HFIR, NRU	ANSTO, CSNS, JRR-3, Dhruva	
low-flux & compact sources	BNC, Kjeller, Delft	Missouri, MNR, LENS, MITR	KURRI, HUNS	Bariloche, SAFARI

Neutron Facility Ecosystem

2025

International "flagship" facilities

ILL | ISIS | SNS

Plenty of action here: STS, ESS, …

regional/national

high-flux & medium-flux scattering facilities

	Europe	North America	Asia	Others
high-flux & medium-flux scattering facilities	MLZ, PSI, ~~LLB~~, ~~HZB~~	NIST, HFIR, ~~NRU~~	ANSTO, Dhruva	
low-flux & compact sources	BNC, Kjeller, ~~Delft~~	Missouri, MNR, LENS, MITR	KURRI	Bariloche

How do we keep this level healthy?

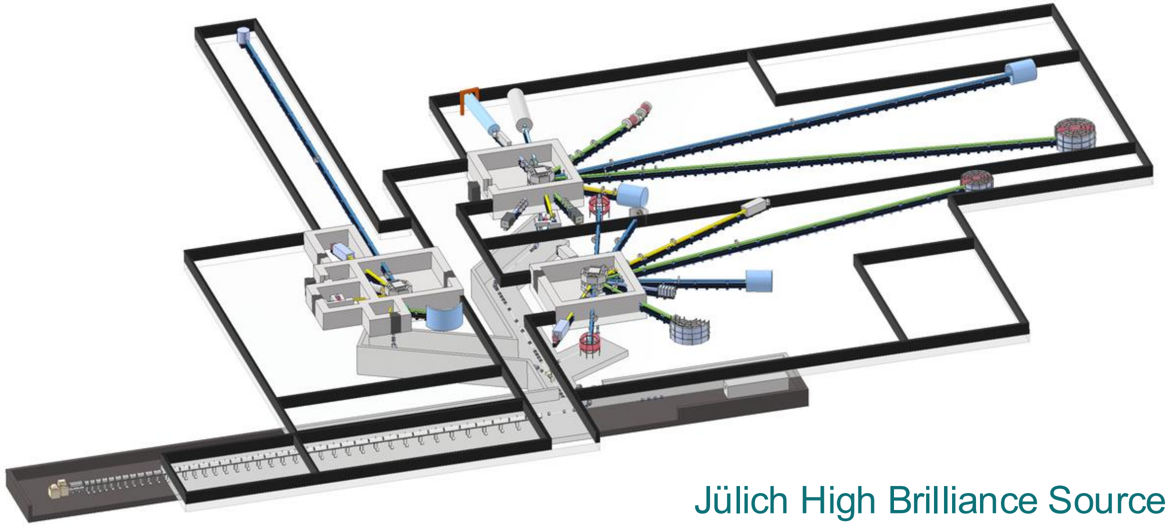
This needs to be boosted!

Approaches for future neutron sources

- Replacement/upgraded research reactors
  - Possible in North & South America, Africa, Asia (partly)
  - Not possible in Europe
- Pulsed Spallation Sources
  - High neutron yield
  - High cost of shielding (particles with energies up to proton energy)
  - Way to go for high-end sources
- Low-energy accelerator-based sources
  - Cheaper proton accelerator (below spallation threshold)
  - Intrinsically lower neutron yield
  - Much cheaper to shield (fewer high-energy particles)
  - Actively pursued in Europe (Germany, France, Spain) and Canada

“Compact” Neutron Sources

- Pulsed proton accelerator
  - Low energy: 2-70 MeV (~1GeV for spallation)
  - Beam power 1-100 kW
  - Well-suited to multiple target stations



Jülich High Brilliance Source

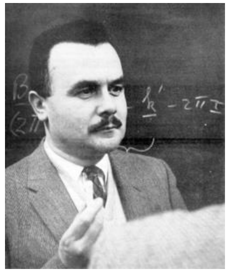
0.01 kW	0.1 kW	1 kW	10 kW	100 kW
0.001-0.01 mA	0.01-1 mA	0.5-5 mA	1-20 mA	50-100 mA
~10^{11} n/s	~10^{12} n/s	~10^{13} n/s	~10^{14} n/s	~10^{15} n/s

10 Mio EUR → 400 Mio EUR

SNS: 1.8 MW
~10^{17} n/s

- Lower-flux facilities are often not user facilities
  - Lower throughput: access through collaboration
  - Develop expert users
  - In-house groups develop new techniques
  - *Train neutron specialists & users*

Students – essential in growing the user community and training next generation neutron scientists.
- Brockhouse and Shull recognized this!



Bert Brockhouse

Chalk River Laboratories

↓

McMaster University (1962)

McMaster Nuclear Reactor
(5 MW - 1959)

Oak Ridge National Laboratory

↓

MIT (1955)

Cliff Shull

MIT Nuclear Research Reactor
(5 MW 1958-1974
6 MW 1974 – present)

Legacy of training students

Students of Bertram Brockhouse

Bill Kamitakahara
Developed the NCNR user program

Eric Svensson
Chalk River – pioneering work on liquid He

Sow-Hsin Chen
Professor MIT

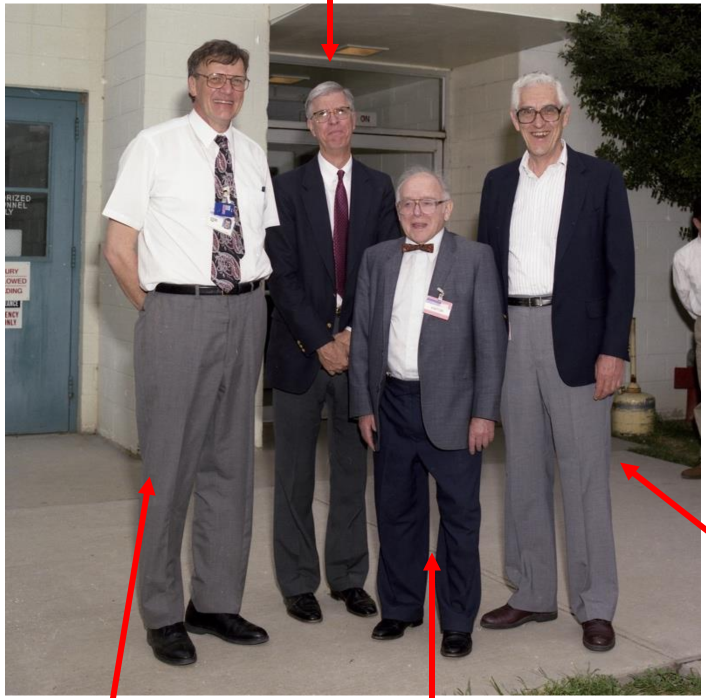
Michael Rowe
Director of NIST Center for Neutron Research

Brockhouse

John Copley
Built DCS spectrometer at NCNR

Students of Clifford Shull

Herb Mook
Pioneering work on superconductors and metals. Former director of neutron scattering at HFIR



David Moncton
Former director of APS and the SNS project

Ralph Moon
Development of neutron polarization analysis. Former director of neutron scattering at HFIR

Shull

Stephen Spooner
HFIR – materials science and residual stress

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Graduate Student Opportunities

Program details: https://education.ornl.gov/gro/

ORNL offers graduate students the opportunity to pursue collaborative research projects with scientists at HFIR and SNS.

The program is open to graduate students from US-based universities admitted to PhD candidate programs. Students are required to apply jointly with their PhD supervisor and an ORNL Neutron Sciences staff member who also will serve as the student’s scientific mentor.

Positions are awarded to work for periods between 3 and 12 months. The students’ salary and benefits are be paid by their university while ORNL covers the costs for allowable travel and local living expenses.

Bottom Line

- Neutron scattering invented the User Facility
  - A large and diverse user community can access facilities which are scientifically essential, but unaffordable to university groups or industry
- It continues to evolve
  - Couple beamtime access with ancillary capabilities: deuteration, sample environment.
  - Provide access to advanced data analysis approaches, HPC, and AI / ML.
- Neutron science relies on healthy ecosystem of neutron facilities
  - International “flagship” facilities
  - National / regional user facilities
  - Compact facilities for training and technique development
- Students are critical to the growth of the neutron user community

Thank you!