Neutron User Facilities

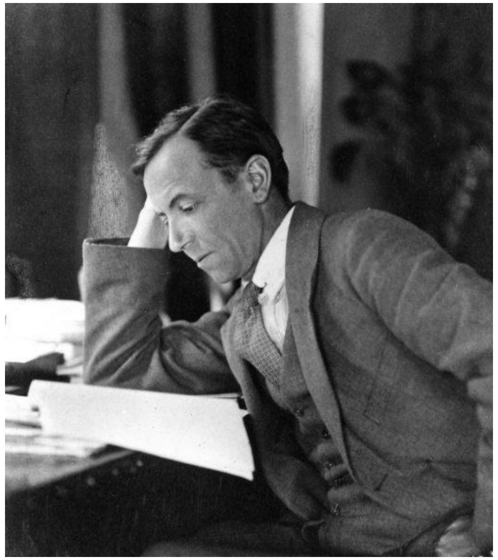
24th National School on Neutron and X-Ray Scattering

July 13, 2022

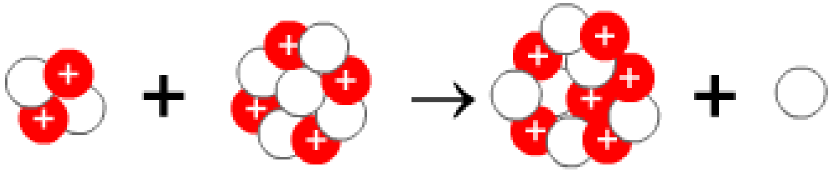
Mark Lumsden

The first neutron source

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

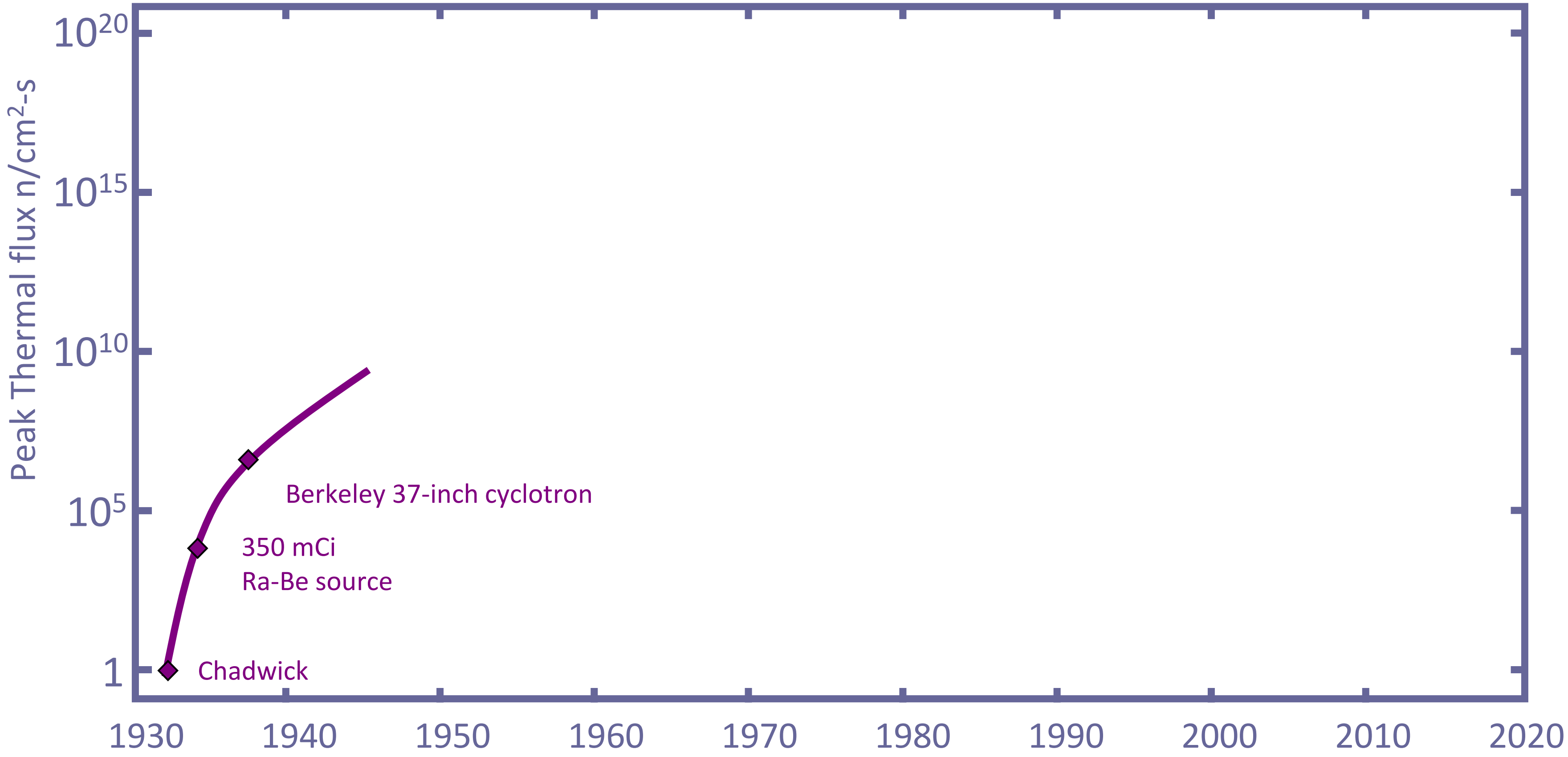


James Chadwick:
used Polonium as alpha emitter on Beryllium



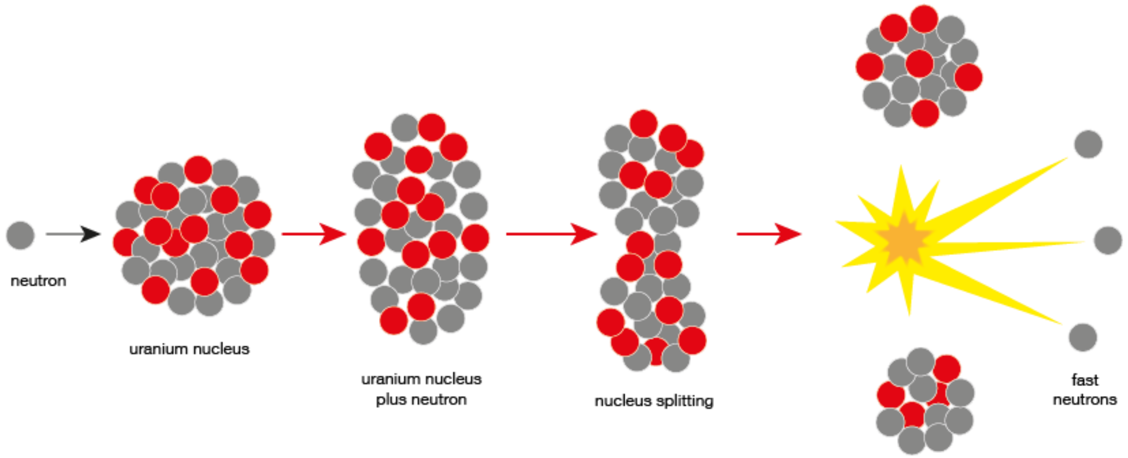
$$^{4}He + {}^{9}Be \rightarrow {}^{12}C + \text{neutron}$$

Evolution of neutron sources



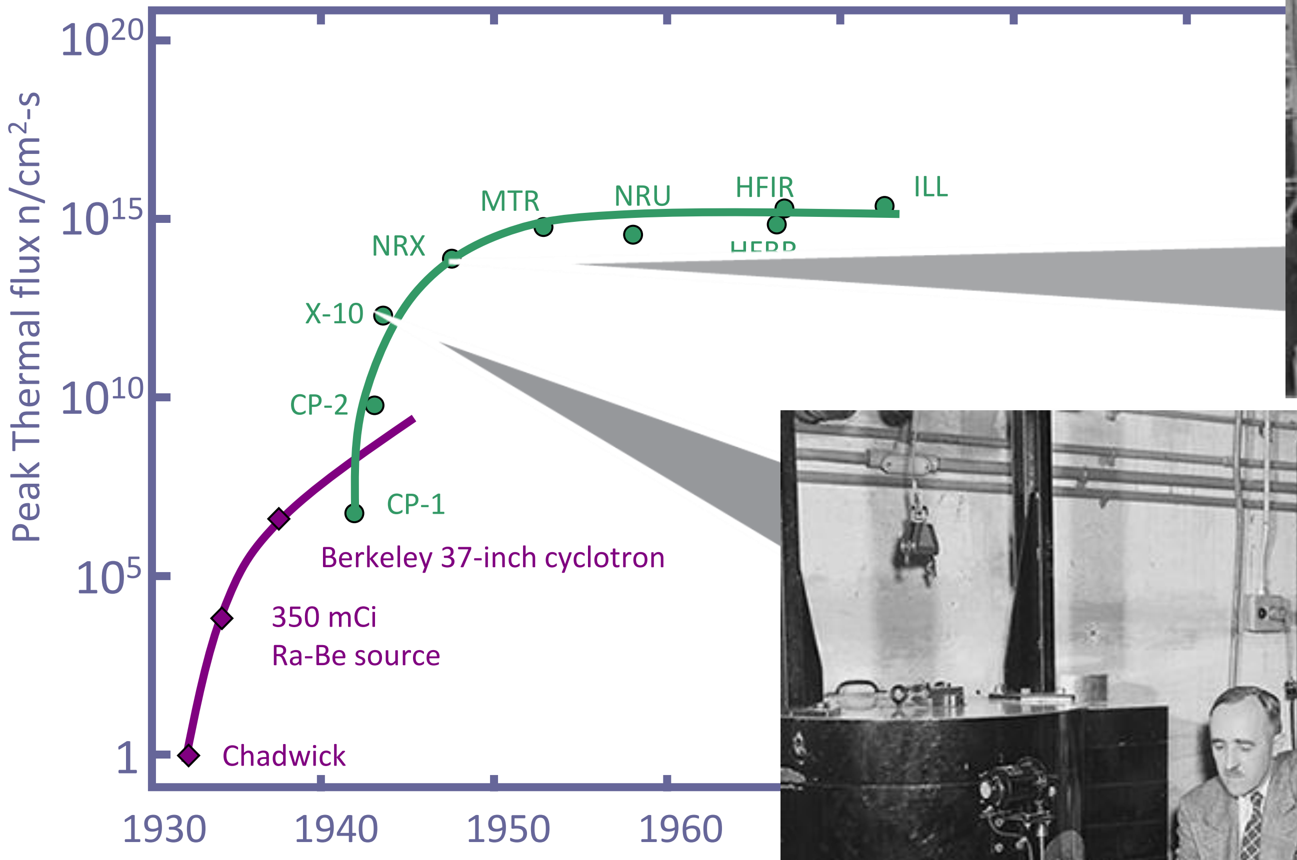
(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

Nuclear fission



200 MeV/fission
2.35 – 1 = 1.35 neutrons freed
⇒ 150 MeV/neutron

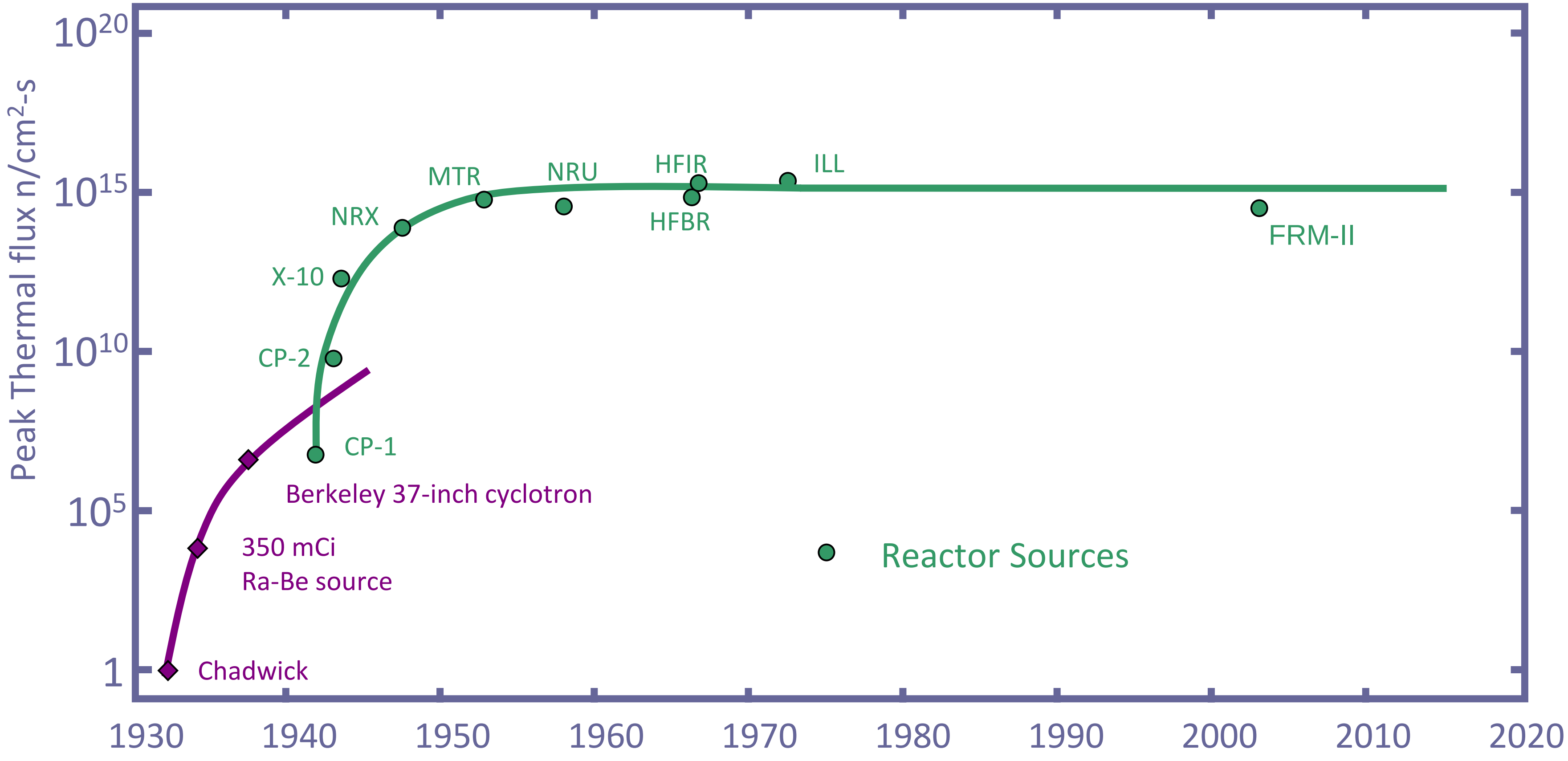
Evolution of neutron sources



(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"

Evolution of neutron sources



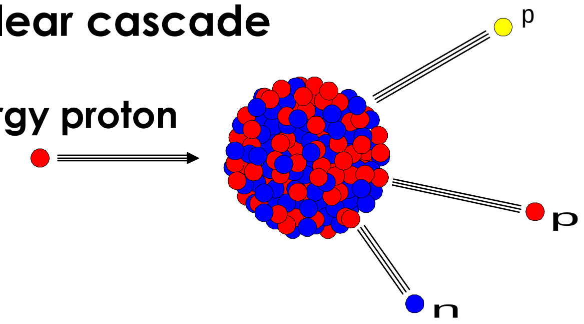
(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

Nuclear spallation

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

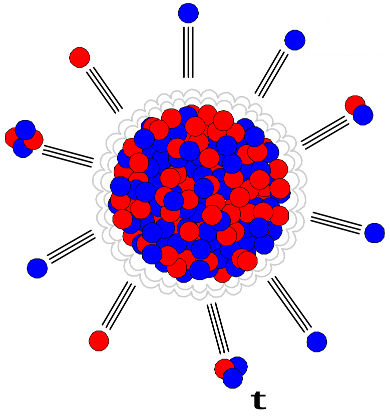
First stage: intranuclear cascade

high-energy proton

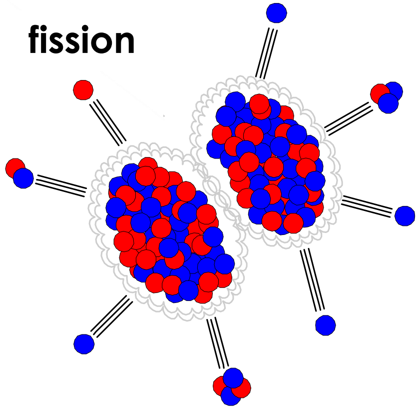


Intermediate stage: pre-equilibrium

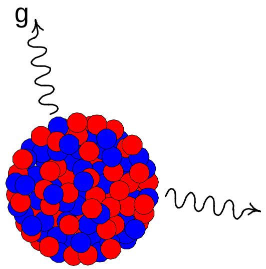
evaporation



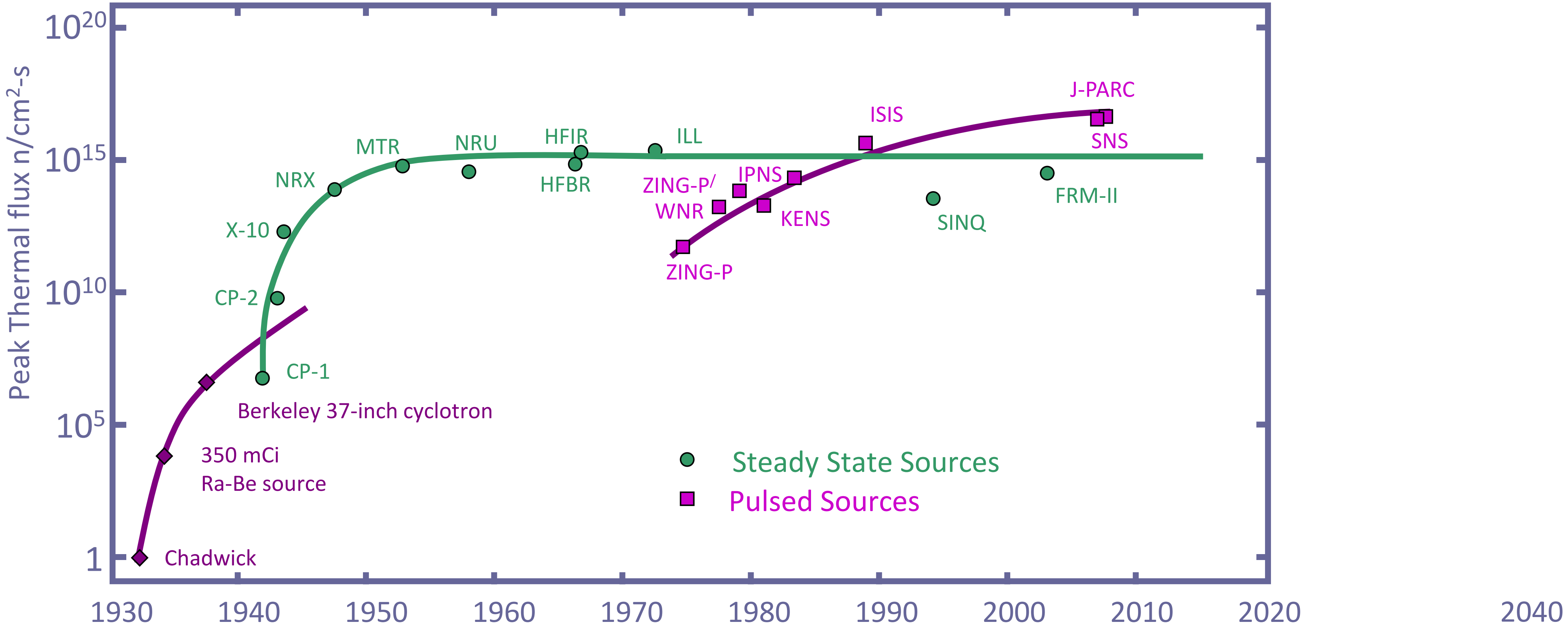
fission



Final stage: residual de-excitation



Evolution of neutron sources



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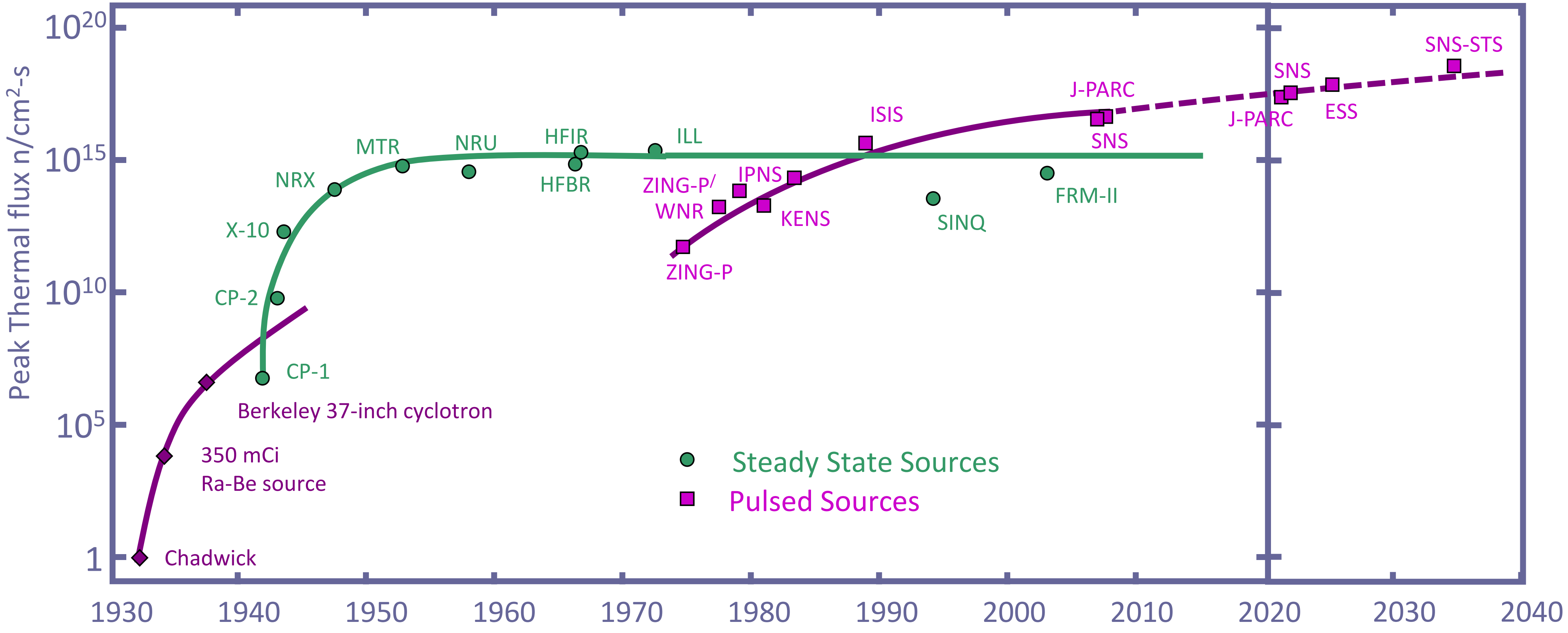
Evolution of neutron sources



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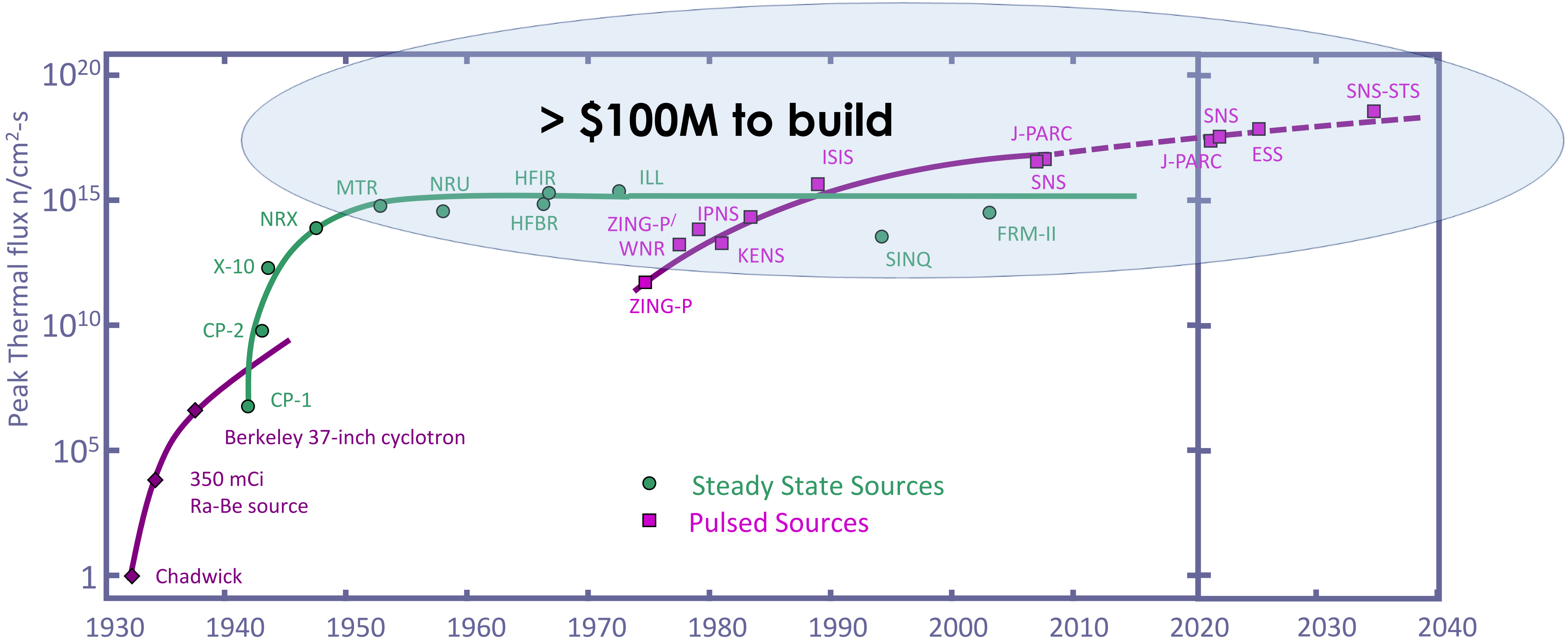
Evolution of neutron sources



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

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

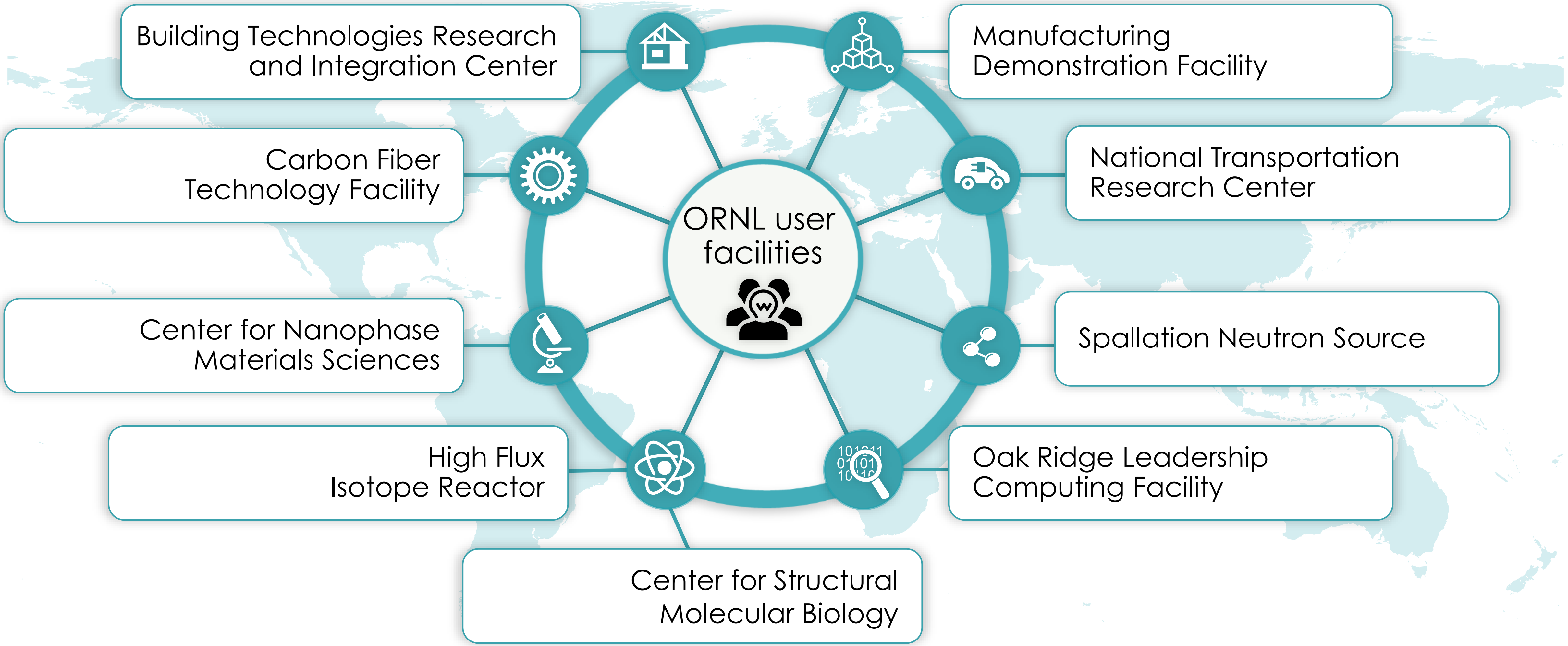
Office of Science User Facilities List:

- 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**

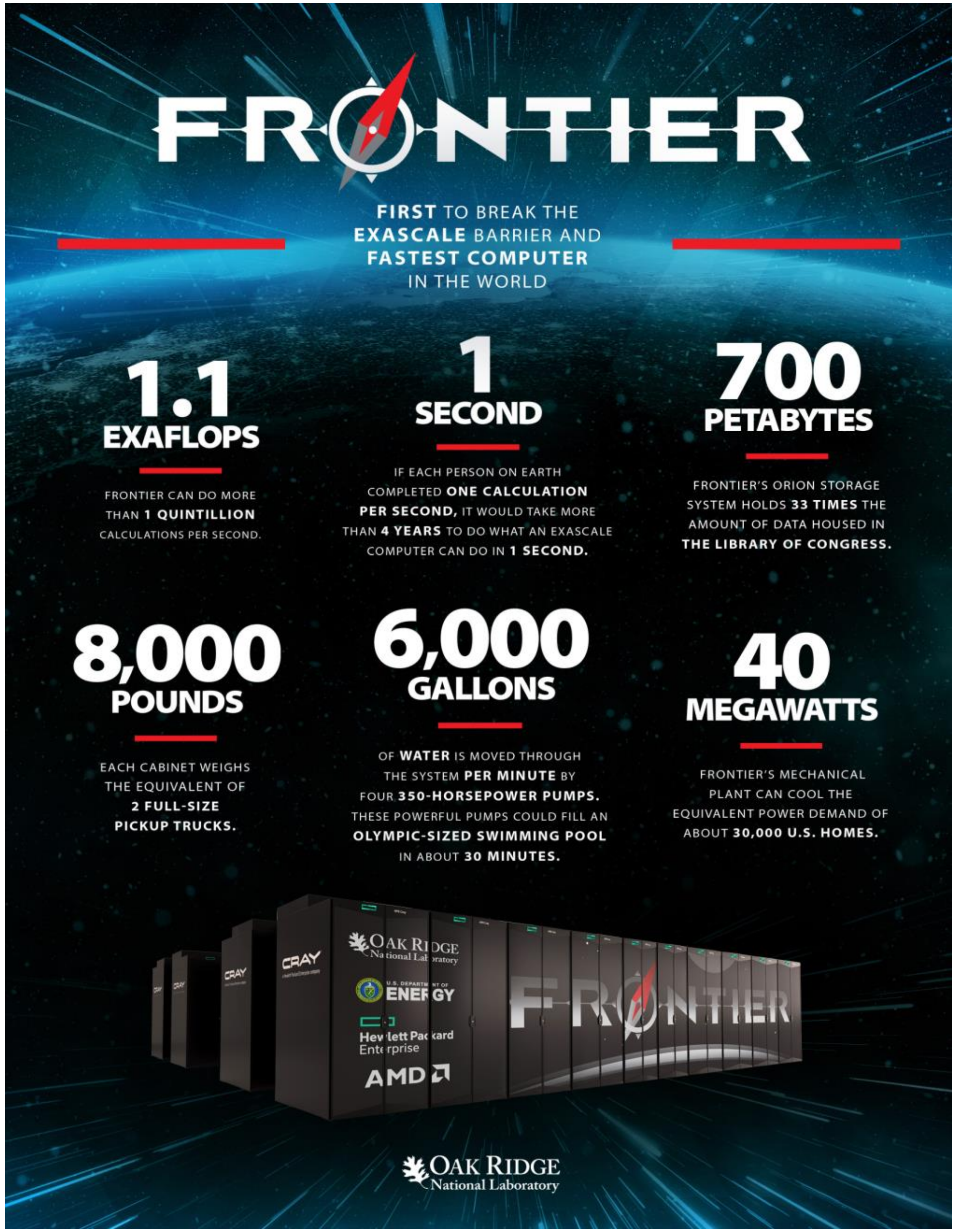
28 Office of Science User Facilities

Oak Ridge National Laboratory User Facilities



Oak Ridge Leadership Computing Facility

- Computing and Computational Sciences Directorate (CCSD) houses the Oak Ridge Leadership Computing Facility, home to ***Summit*** and now ***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
- Access to OLCF resources is limited to approved projects and their users through user proposals and depends on the scientific merit, suitability and appropriateness of work to DOE objectives.



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

TOP500 LIST - JUNE 2022

R_{max} and R_{peak} values are in PFlop/s. For more details about other fields, check the TOP500 description.

R_{peak} values are calculated using the advertised clock rate of the CPU. For the efficiency of the systems you should take into account the Turbo CPU clock rate where it applies.

← 1-100 | 101-200 | 201-300 | 301-400 | 401-500 →

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90	214.35	2,942
4	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
5	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94.64	125.71	7,438

Center for Nanophase Materials Sciences

A user facility for nanoscale and quantum materials

- **Broad spectrum of imaging capabilities**
  - scanning transmission electron microscopy 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.

Neutron User Facilities in North America

High Flux Isotope Reactor (HFIR)

Operating at 85 MW, HFIR provides one of the highest steady-state neutron fluxes of any reactor in the world for materials research.

12 Instruments in the user program

Spallation Neutron Source (SNS)

SNS is the most powerful pulsed neutron source in the world for materials research

18 Instruments in user program

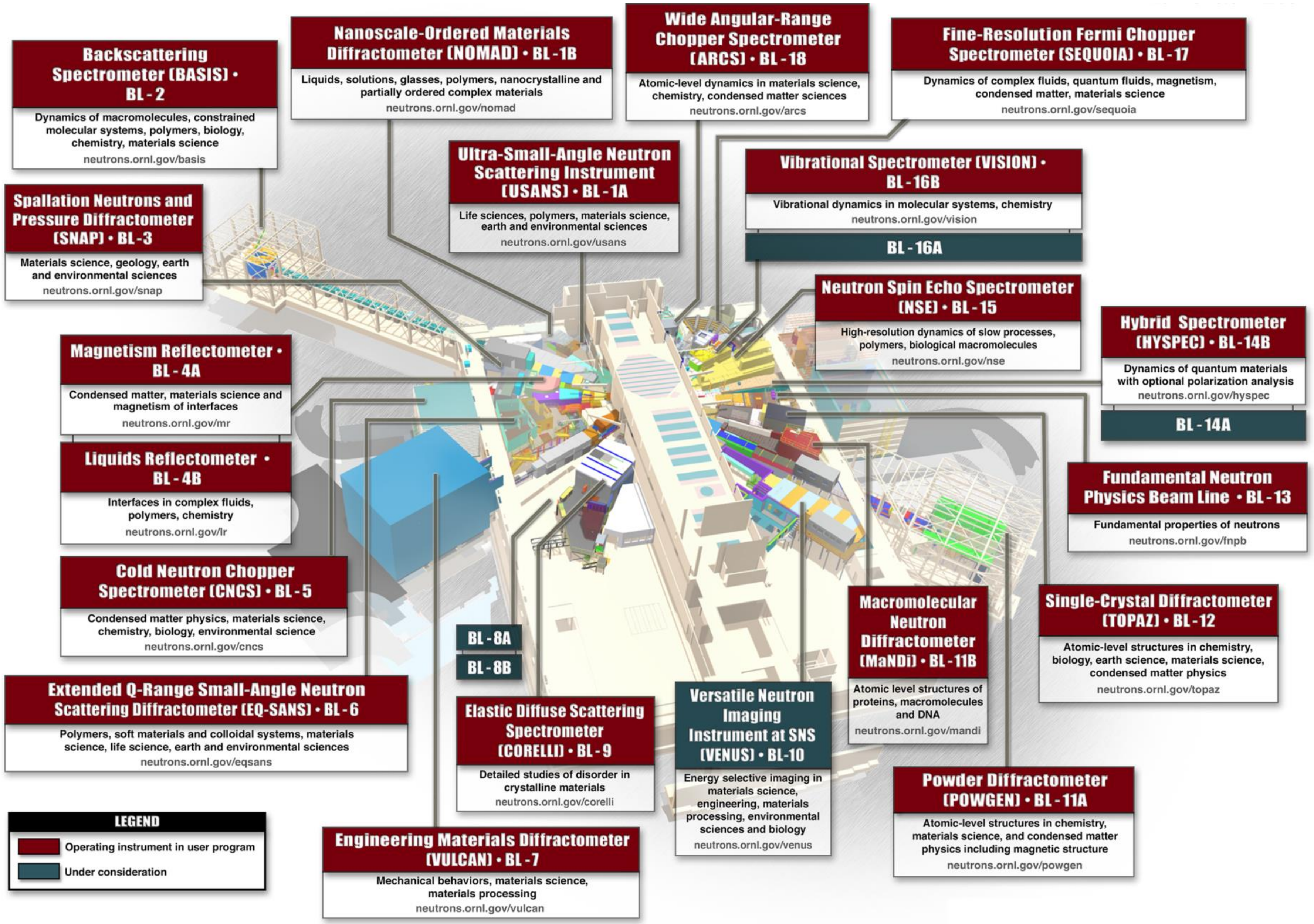
NCNR

20 MW reactor in Gaithersburg, MD

13 Instruments in user program.

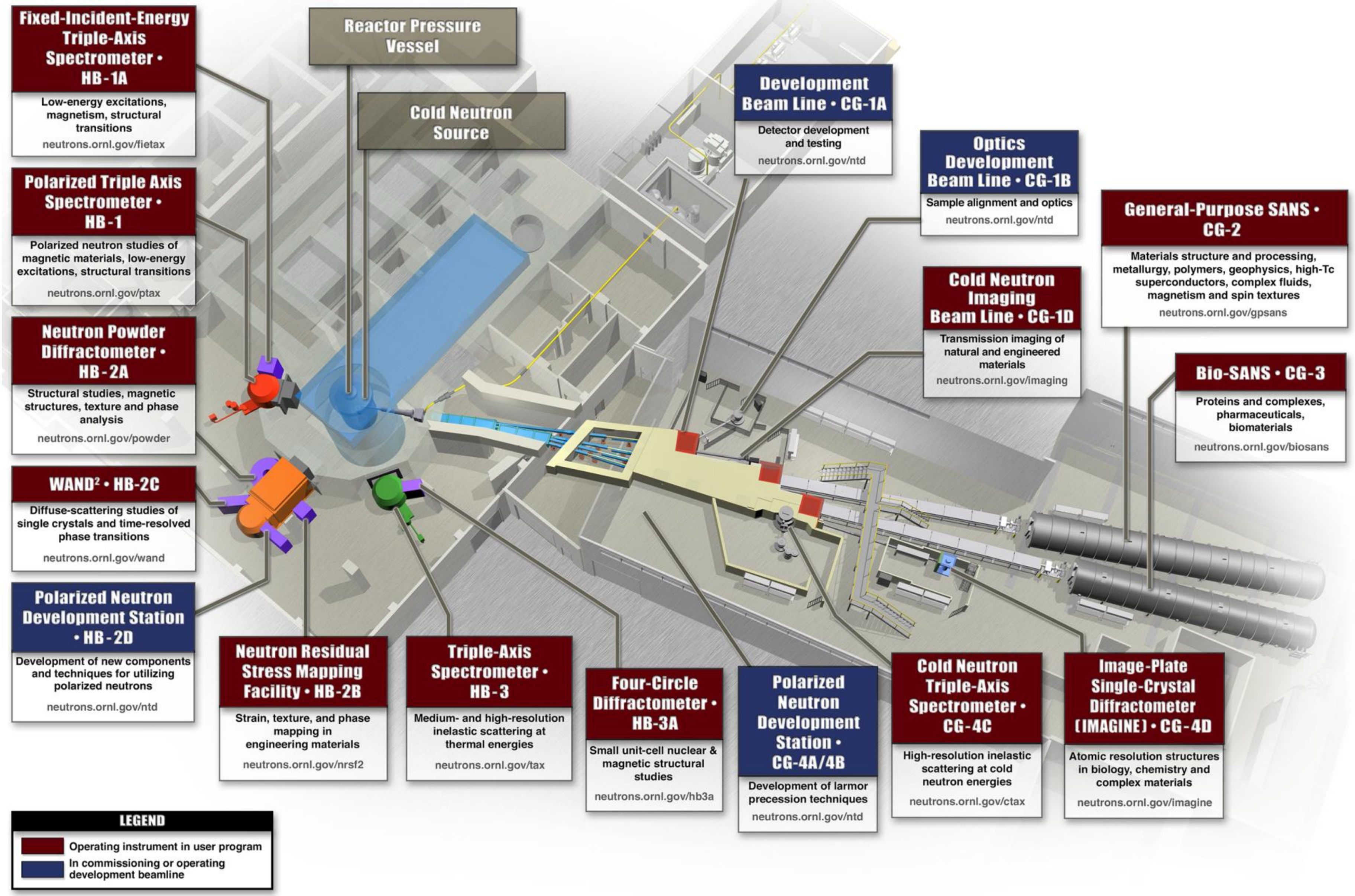
Spallation Neutron Source

- 18 instruments in user program
  - Diffraction
  - Spectroscopy
  - Engineering
  - SANS & reflectrometry
- 1 not in user program
  - Fundamental physics
- 1 instrument in construction
- 4 available instrument slots



High Flux Isotope Reactor

- 12 instruments in user program
  - Diffraction
  - Spectroscopy
  - Engineering
  - Imaging
  - SANS
- 4 development beamlines
- Non-beam program
  - Isotope production
  - Irradiation facilities
  - Activation analysis
  - Fundamental physics



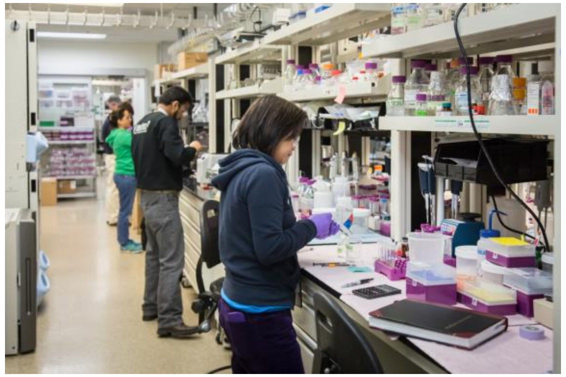
Becoming a neutron scattering user at SNS or HFIR

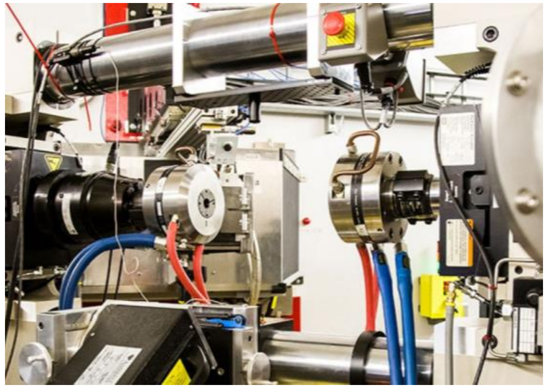
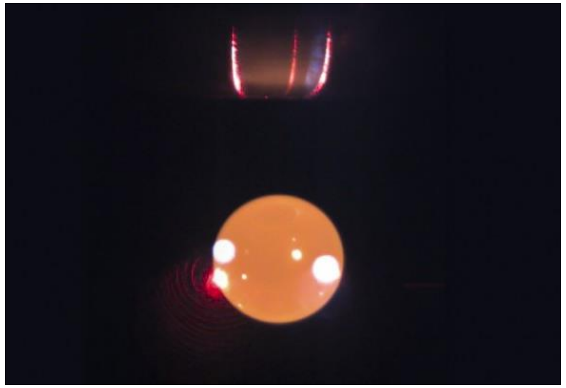
- Prospective users should submit a proposal to one of our biannual proposal calls
- 2022 proposal call deadlines are March 23 and September 21
- 1500+ General User proposals requesting beam time are received annually

- 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

Sample Environment and Complementary Facilities



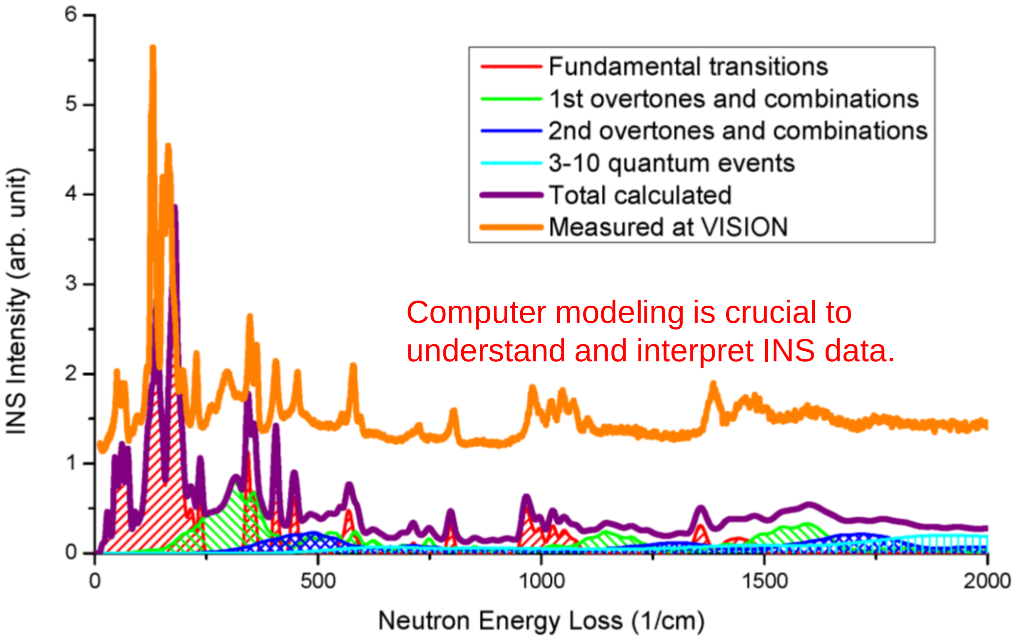


Experiments are increasingly complex – few ‘routine’ measurements

Complementary laboratory facilities are needed for sample preparation (including deuteration) and characterization

Integrated Modeling (VISION)

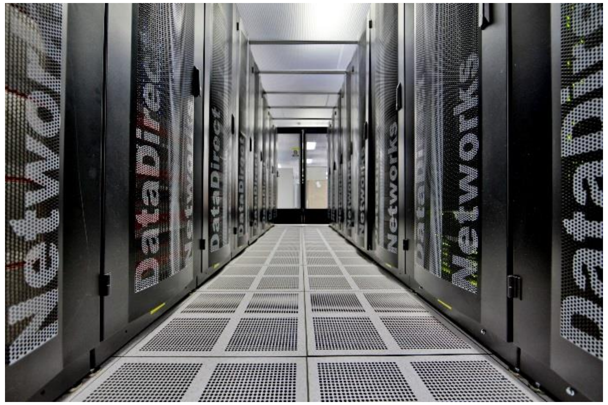


Computer modeling is crucial to understand and interpret INS data.

OCLIMAX

(YQ Cheng, Timmy Ramirez-Cuesta)

Inelastic neutron scattering calculation for both powders and single crystals using DFT



VirtuES cluster

QUANTUM ESPRESSO

Vienna Ab-initio Simulation Package

CASTEP

CP2K

ORCA

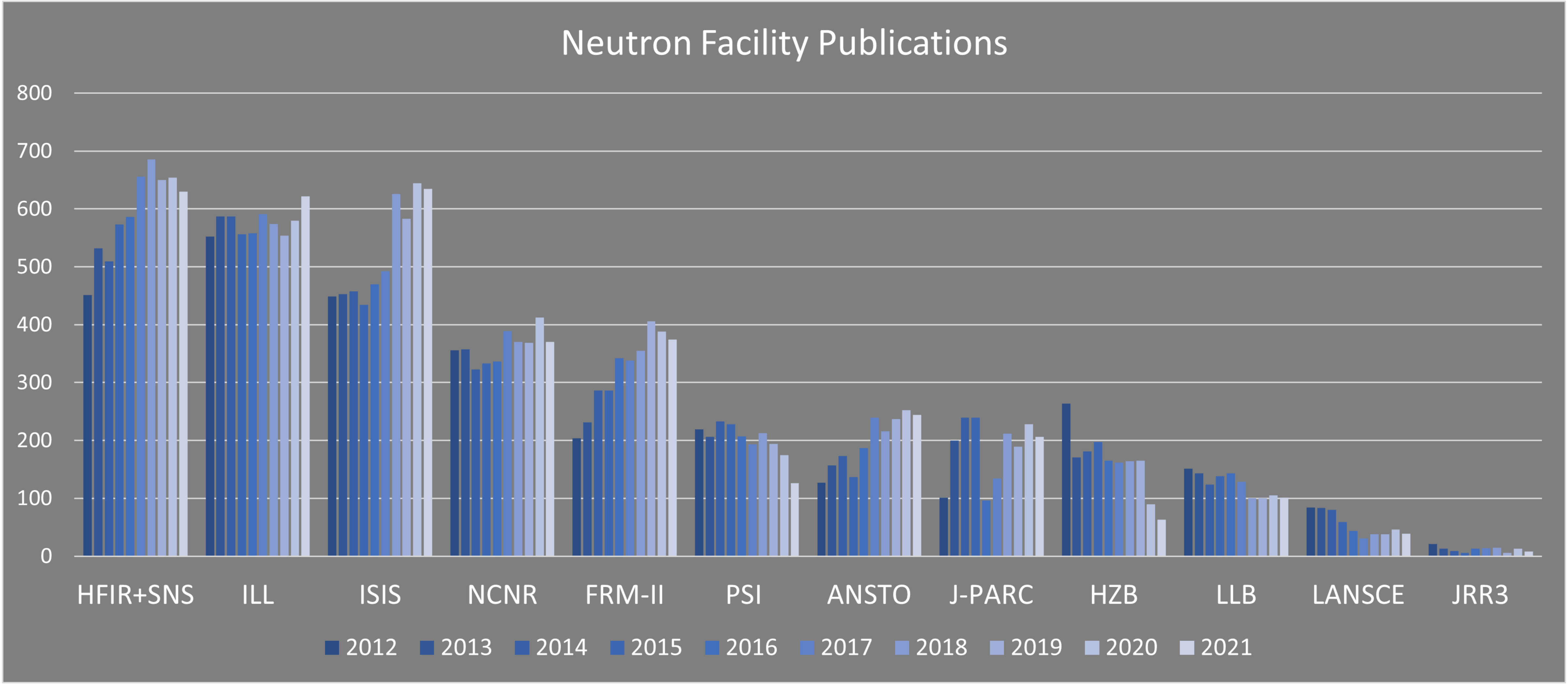
NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

RMG

Neutron User Facilities Worldwide

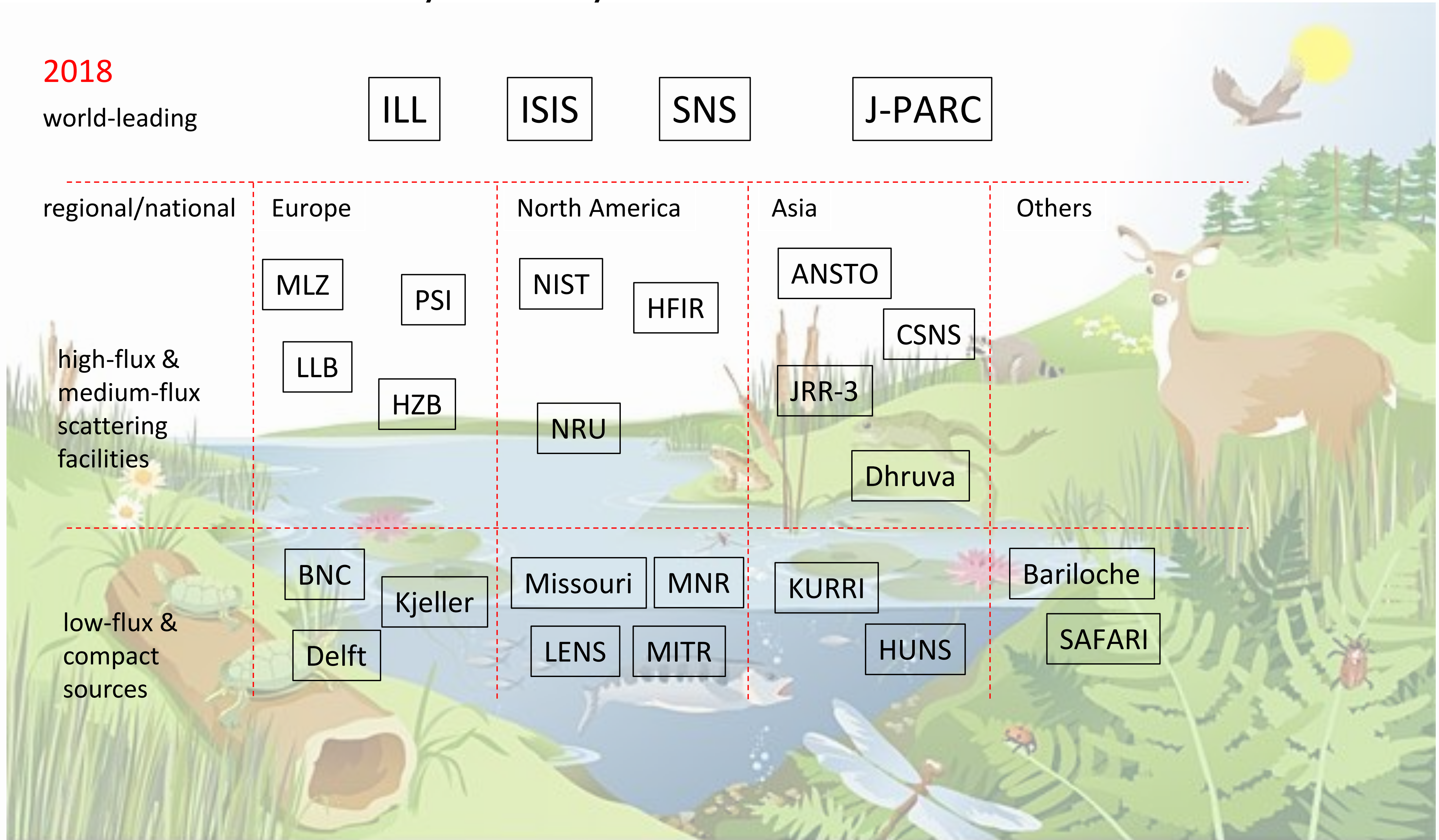
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Neutron Facilities Worldwide



Neutron Facility Ecosystem

Neutron Facility Ecosystem



2018

	Europe	North America	Asia	Others
world-leading	ILL, ISIS	SNS	J-PARC	
regional/national: 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

2022

world-leading: ILL, ISI…

Plenty of action here: STS, ESS, …

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

How do we keep this level healthy?

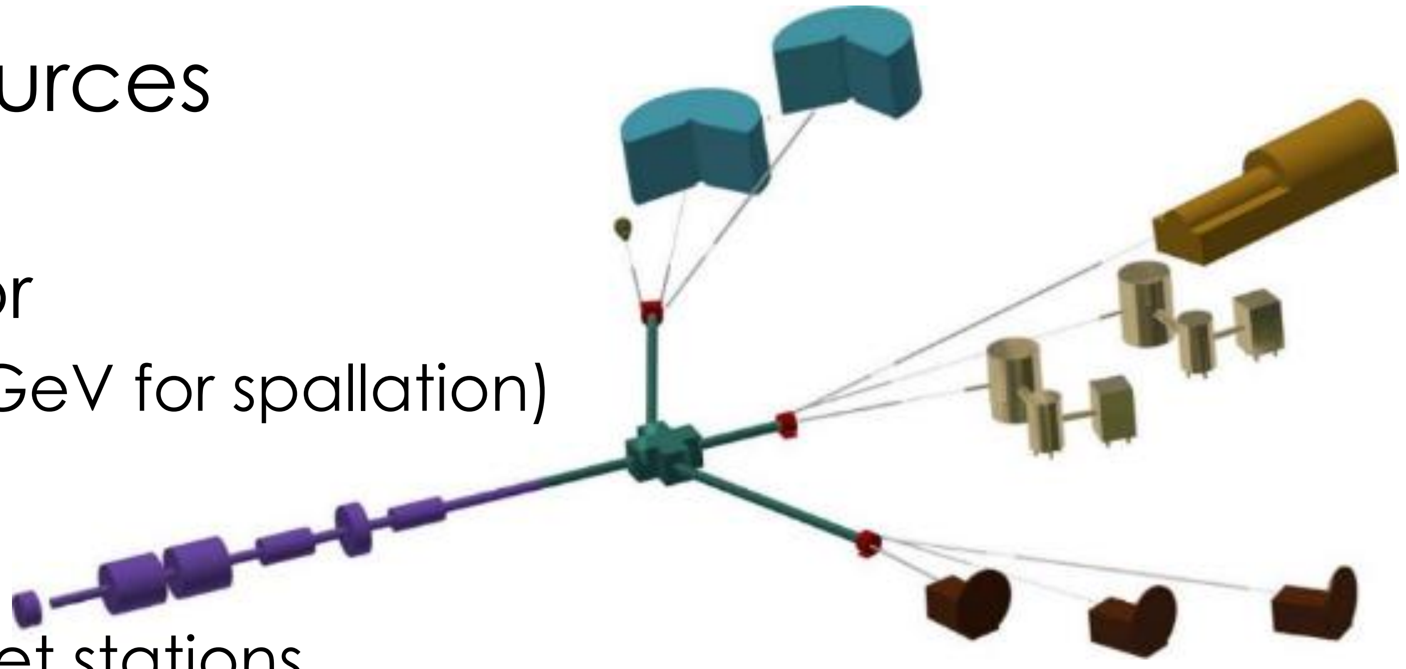
This needs to be boosted!

Approaches for future neutron sources

- Replacement/upgraded research reactors
  - Doable in North & South America, Africa, Asia (partly)
  - Not doable 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)
  - 1-4% duty cycle
  - Beam power 1-100 kW
  - Well-suited to multiple target stations
  - Scaleable



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
$\sim 10^{11}$ n/s	$\sim 10^{12}$ n/s	$\sim 10^{13}$ n/s	$\sim 10^{14}$ n/s	$\sim 10^{15}$ n/s

10 Mio EUR → 400 Mio EUR

SNS: 1.4 MW
$\sim 10^{17}$ n/s

“Compact” Neutron Sources

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

Bottom Line

- Neutron scattering invented the User Facility
  - Effective and efficient means of providing access to large and diverse user community
  - Access to facilities which are scientifically essential, but unaffordable to university groups or industry
- We're still reinventing it
  - Couple beamtime access with ancillary capabilities: deuteration, sample environment, advanced data analysis approaches, …
- Neutron science relies on healthy ecosystem of neutron facilities
  - High-end user facilities
  - Medium-flux hybrid user facilities
  - Compact facilities doing collaborative science

Thank you!