26th National School on Neutron and X-ray Scattering

Stephen Streiffer
Laboratory Director,
Oak Ridge National Laboratory

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Many many thanks to…

Jonathan Lang
Argonne National Laboratory
Light source slides

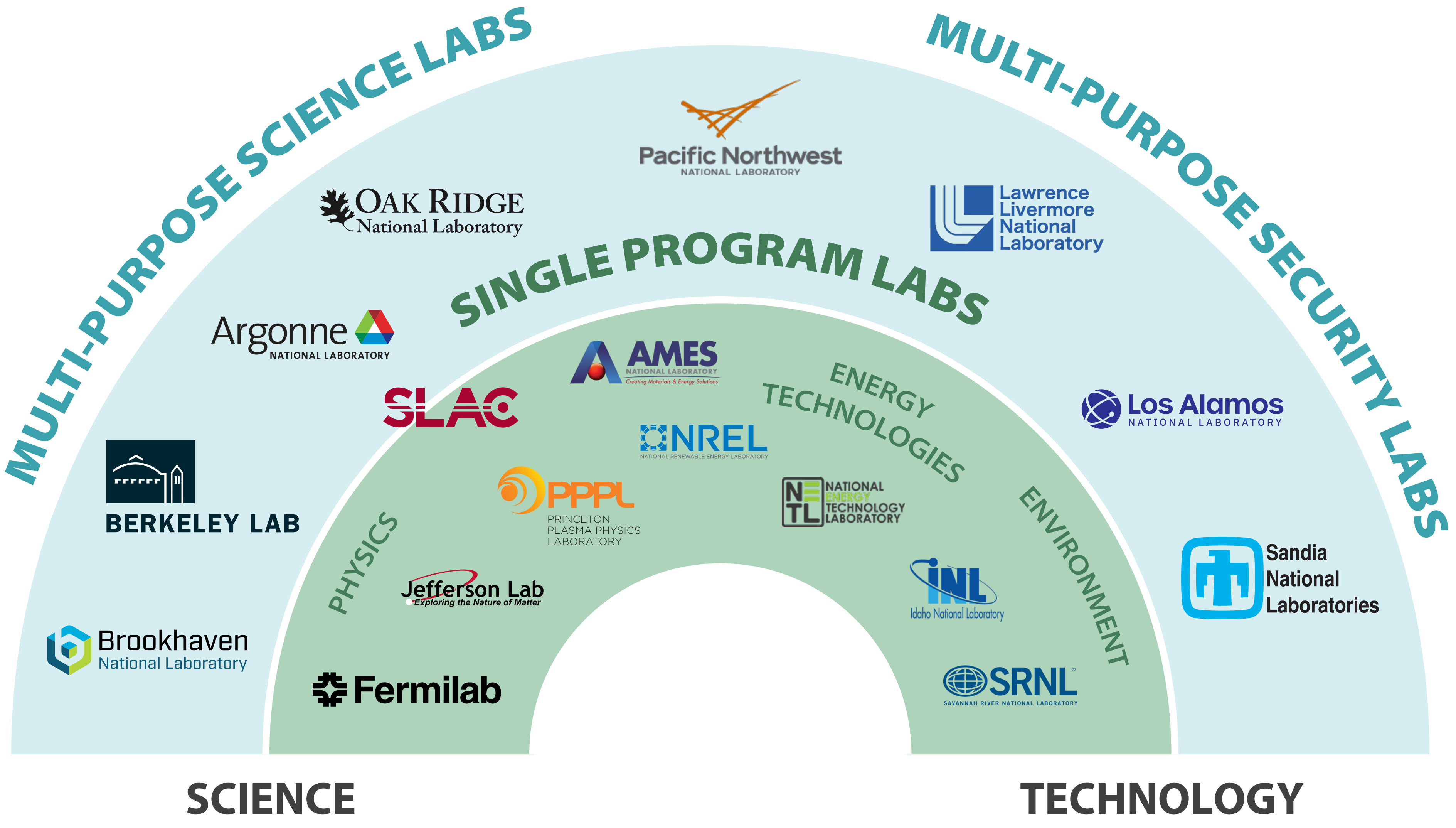
Mike Dunne
SLAC National Accelerator Laboratory
XFEL slides

Mark Lumsden
Oak Ridge National Laboratory
Neutron slides

Outline

1. Introduction and comparison of X-ray and neutron sources
2. Storage ring light sources and X-ray free electron lasers
3. Neutron sources

DOE executes its missions through diverse national labs

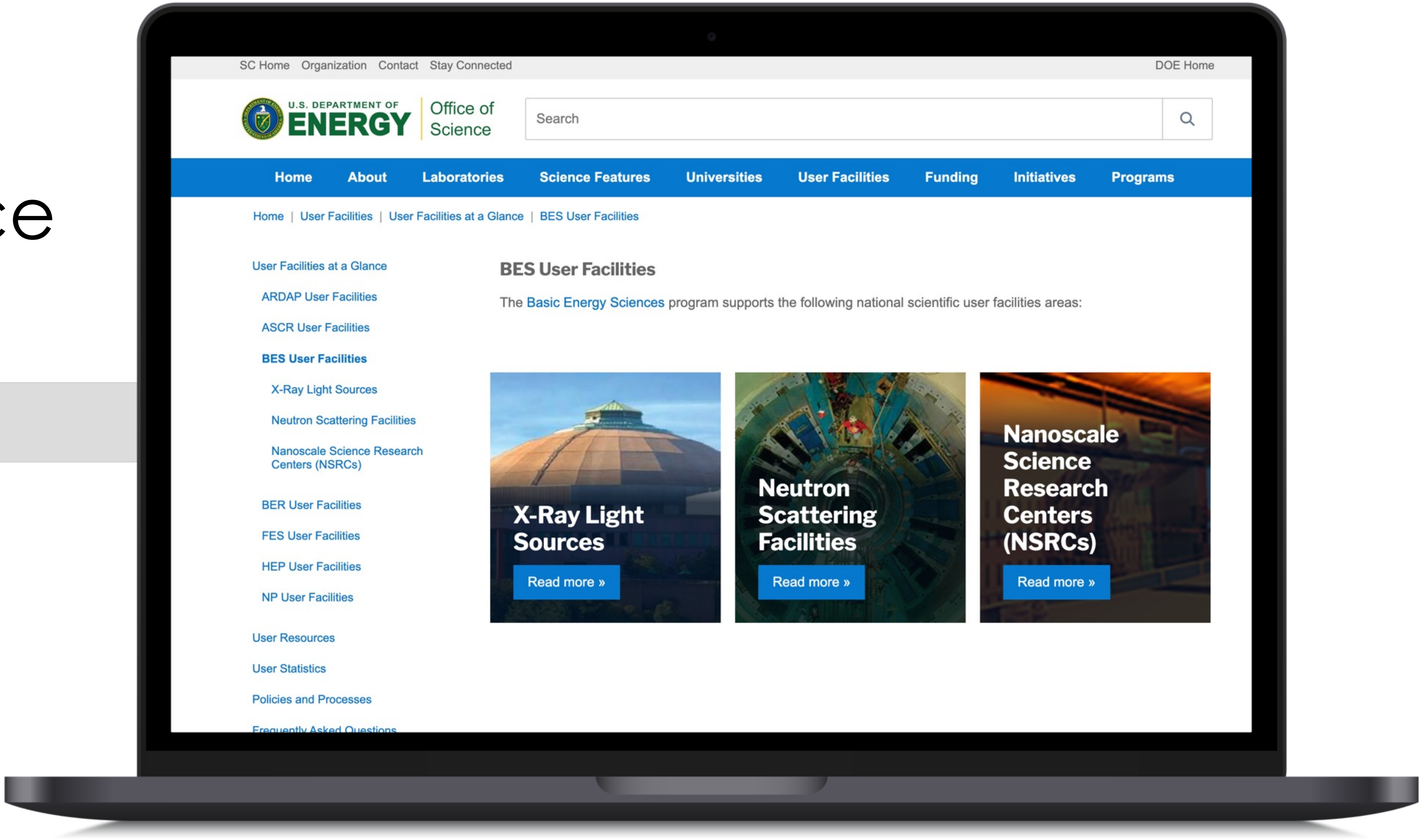


Oak Ridge National Laboratory

Office of Science user facilities

Basic Energy Sciences supports light sources and neutron scattering facilities

- energy.gov/science/office-science-user-facilities
- science.osti.gov/User-Facilities/



User facilities are open to the research community

Why the Office of Science and National Labs?

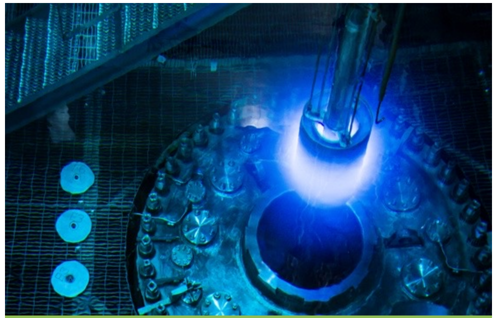
- **Importance of technique**
- **High cost of facility**
- **Key enabler of "small science"**
- **Now a widespread business model in science**

User facility management

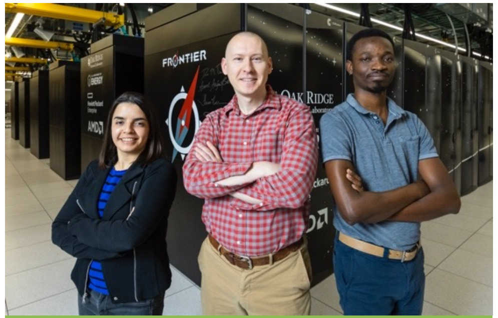
- Open to all without regard to nationality or affiliation
- Access based on merit review
- Free to use if results are to be published
- Facility allows safe and efficient work
- Facility supports user organization to represent users and promote collaboration
- Facility does not compete with private sector capability

Oak Ridge National Laboratory user facilities

Center for Nanophase Materials Sciences



High Flux Isotope Reactor



Oak Ridge Leadership Computing Facility

Spallation Neutron Source

Building Technologies Research and Integration Center

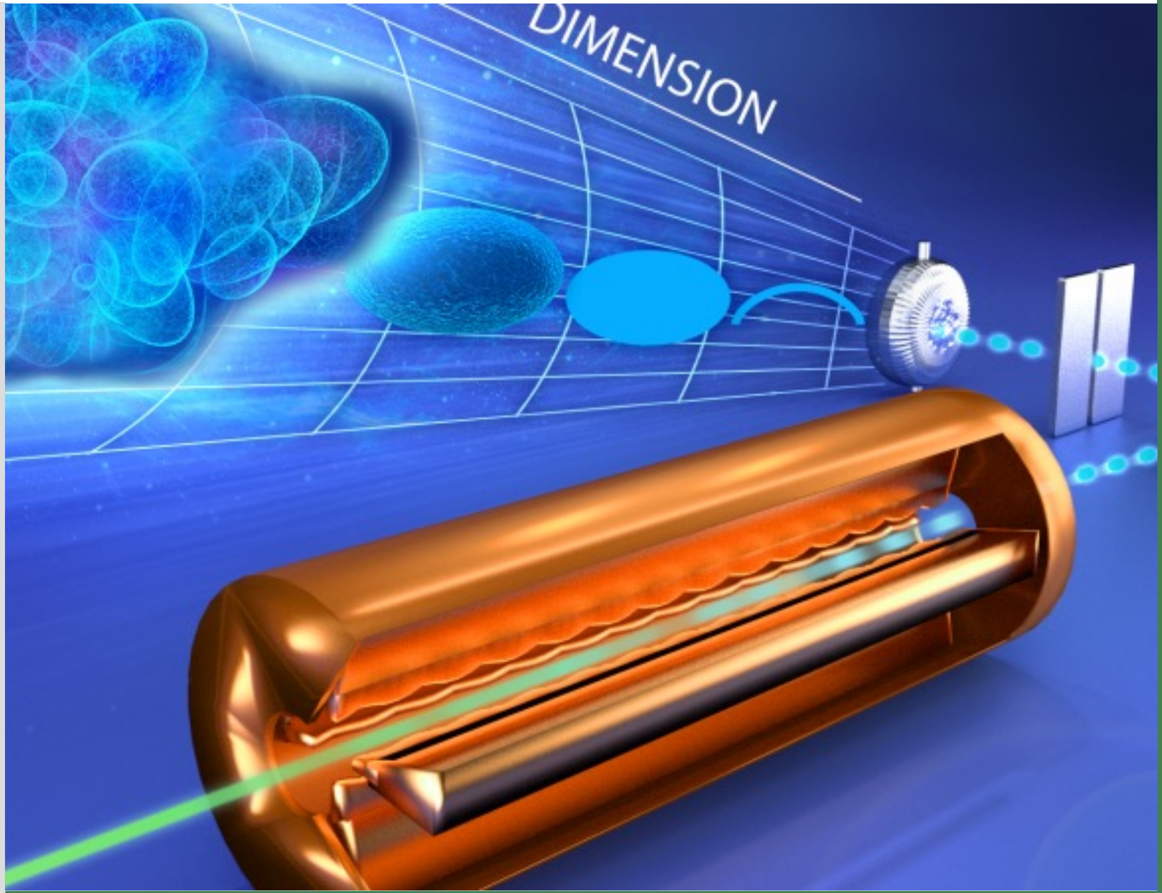
Carbon Fiber Technology Facility

Manufacturing Demonstration Facility

National Transportation Research Center

What quantities characterize a particle beam for a given energy bandwidth?

- **Intensity**: particles per second
- **Fluence**: particles per unit area
- **Flux** (density): particles per second per unit area
- **Brightness**: particles per second per unit area per unit solid angle
- **Brilliance**: intellectual quality of facility staff and users
- **Emittance**: beam position and momentum phase space



X-ray and neutron facilities enable complementary experimental methods

X-rays

Tunable source of photons across range of wavelengths, applicable to different types of experiments

Weakly to strongly penetrating

(Weakly) sensitive to magnetism because X-rays are polarized

Sources can be extremely bright, high flux, and moderately to fully coherent

Sources can produce sub-nanosecond to attosecond pulses for time-resolved studies

Ionizing

Neutrons

Sensitive to light elements and isotopes

Magnetic moment is very sensitive to magnetism

Neutron capture can be a problem for certain samples

Ideal for measuring certain types of electronic band structure/dynamics

Highly penetrating

Sources are not hugely tunable; Sources are comparatively not very bright or very high flux

X-ray sources are much brighter than neutron sources

APS-U

Pinhole Flux (density):
2×10^{15} ph/(0.5mm)^2/sec/0.1%BW

Avg Brightness:
2×10^{22} ph/mm^2/mrad^2/0.1%BW/sec

SNS First Target Station (1Å)

Avg Thermal Flux (density):
2×10^{13} n/cm^2/sec

Peak Thermal Flux (density):
2×10^{16} n/cm^2/sec

Avg Brightness:
10^{12} n/cm^2/sr/Å/sec

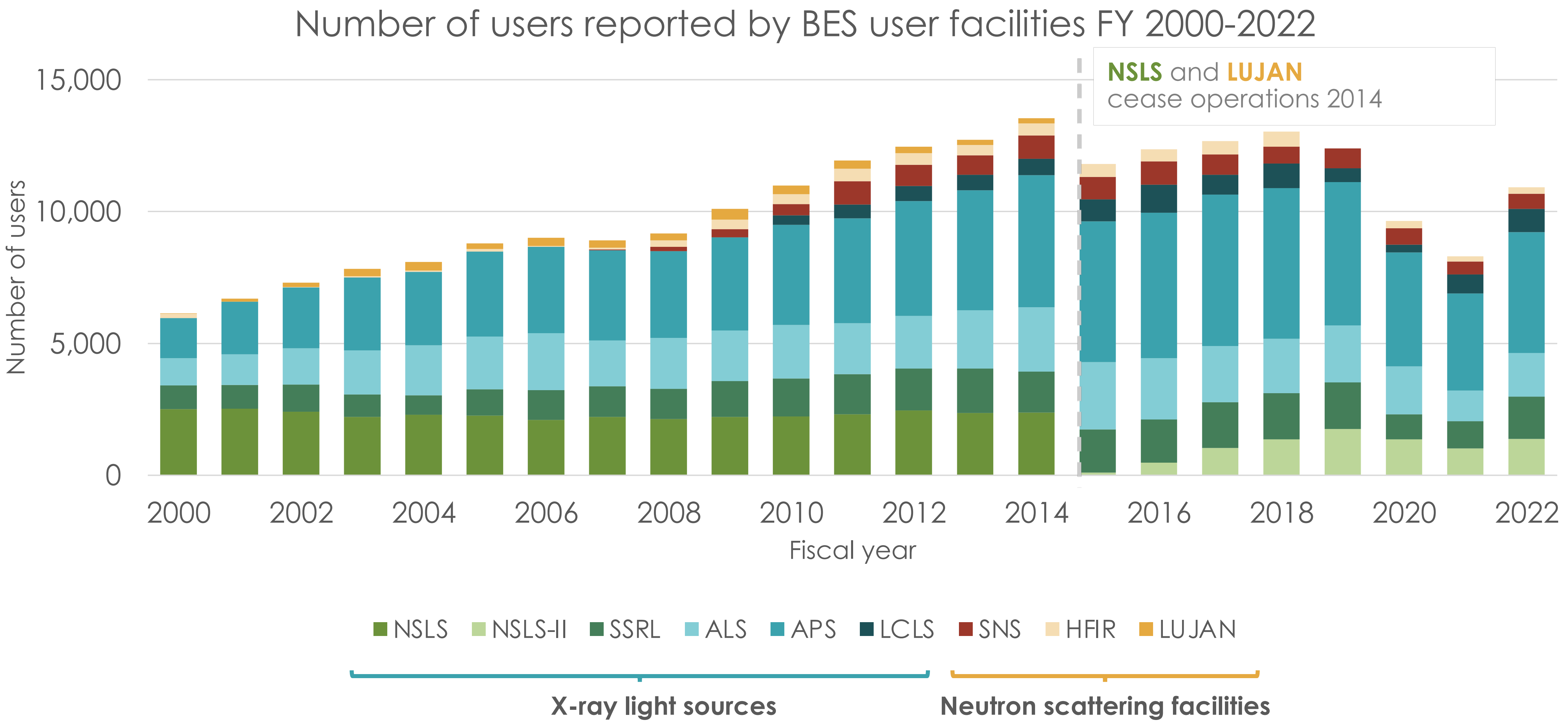
Peak Brightness:
10^{15} n/cm^2/sr/Å/sec

HFIR (1Å)

Avg Thermal Flux (density):
3×10^{15} n/cm^2/sec

Avg Brightness:
5×10^{13} n/cm^2/sr/Å/sec

DOE scientific user facilities



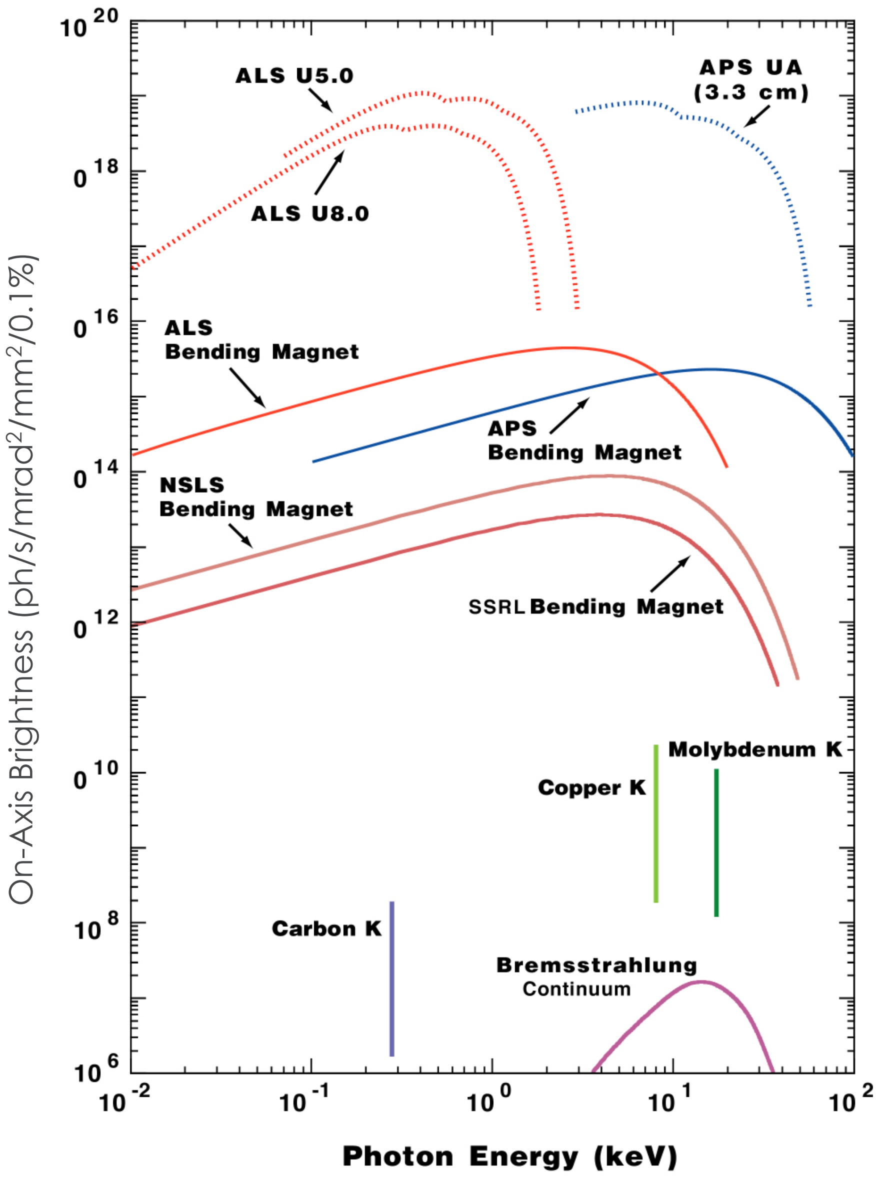
X-ray user facilities

Why use a synchrotron X-ray source?

Synchrotron Radiation (SR) - radiation from the acceleration of a charged particle

$$\text{Brightness} = \frac{\text{Photons/second}}{(\text{mrad})^2(\text{mm}^2\ \text{source area})(0.1\%\ \text{bandwidth})}$$

- $(\text{mrad})^2$ → beam collimation
- $(\text{mm}^2\ \text{source area})$ → size of beam source
- $(0.1\%\ \text{bandwidth})$ → monochromaticity

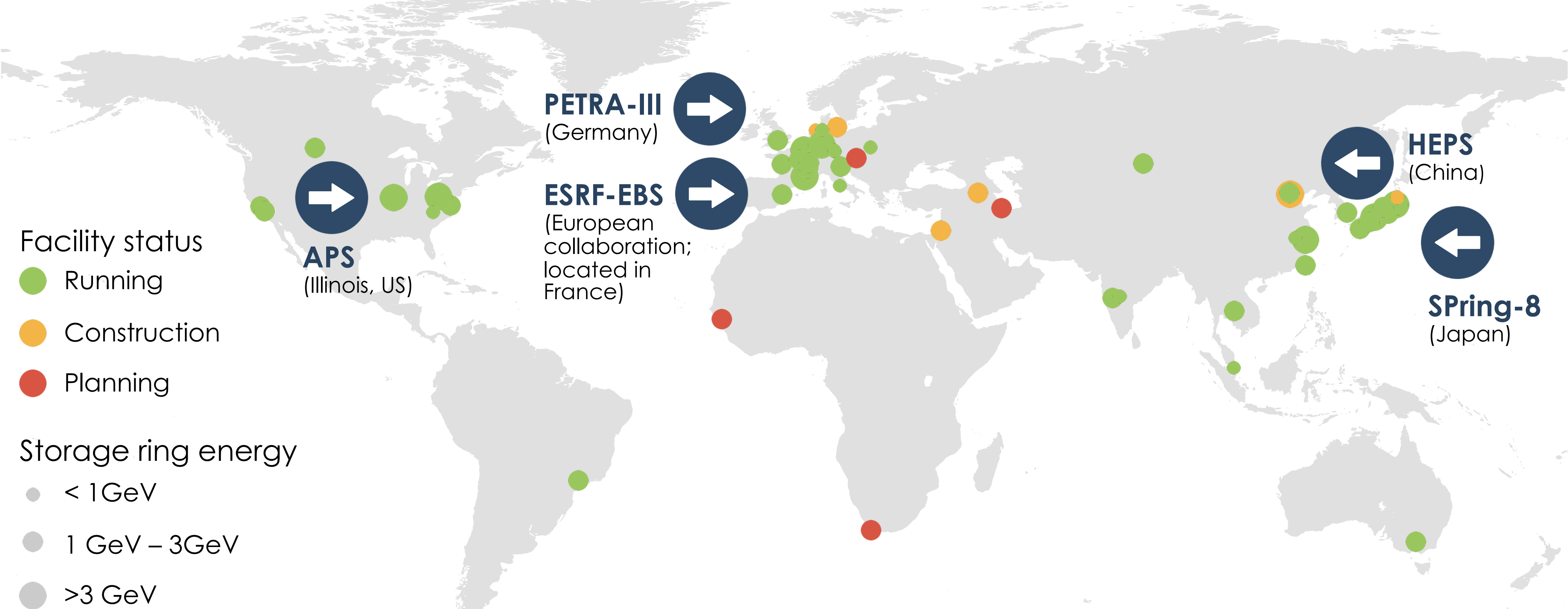


10.97

$\lambda[\text{Å}] = 12.4 / E[\text{keV}]$

Synchrotron facilities around the world

Over 40 synchrotron light-source facilities world-wide



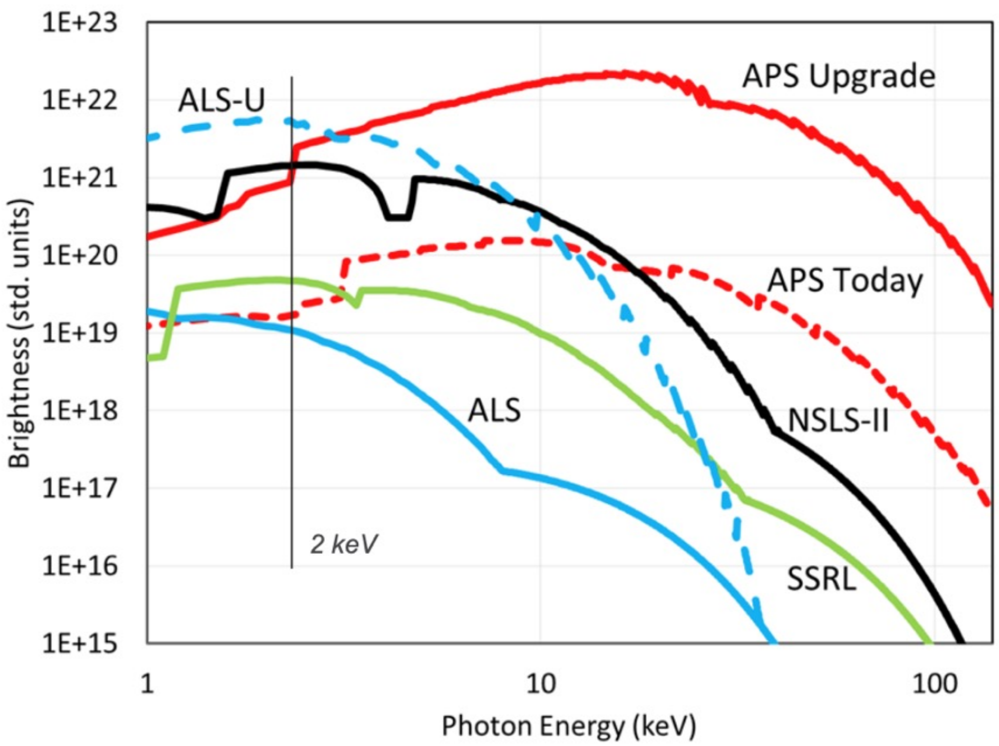
Approximately 50,000 scientists use one of these facilities each year

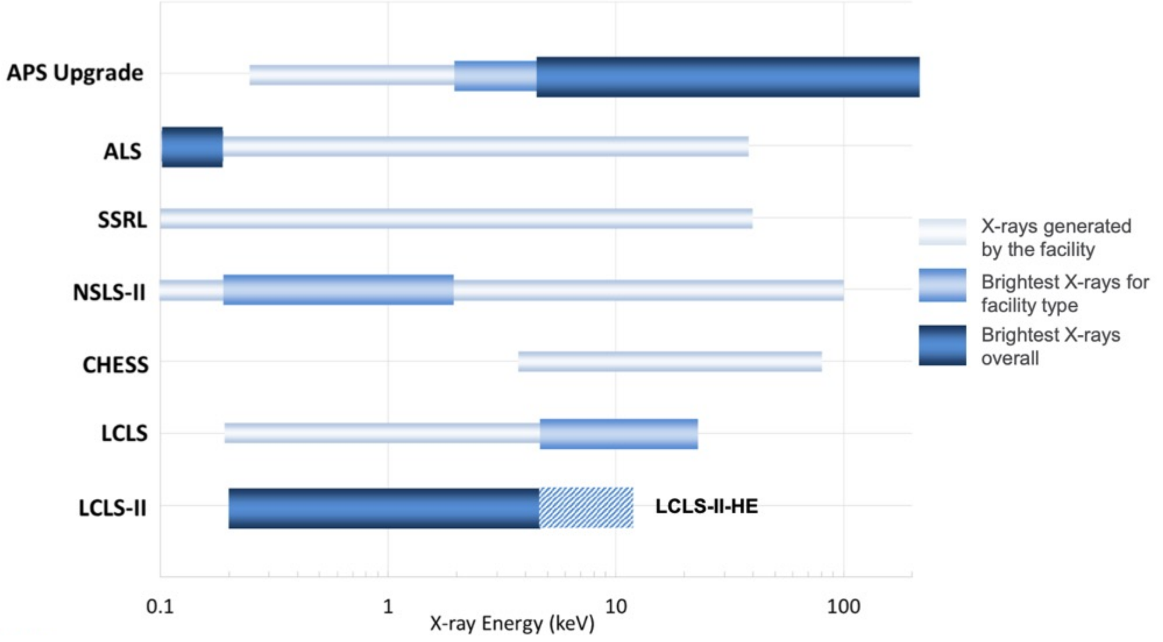
Five are large-circumference high-energy (>5 GeV) high-brightness (<3nm-rad) storage rings

See lightsources.org

DOE light source facilities

Light sources optimized* for particular energy ranges





Harder X-rays contain significant power in the X-ray beam

Lower energy ring can go to higher current without heat load mitigation

Light source parameters

Source	Energy	Current	Circum.	Emittance	# Beamlines
APS	7.0 GeV	100 mA	1104m	3.0 nm-rad	67 (47 ID)
APS-U	6.0 GeV	200 mA	1104m-d	0.042 nm-rad	70 (54 ID)
NSLS-II	3.0 GeV	400 mA	792m	0.75 nm-rad	30 (22 ID)
SSRL	3.0 GeV	500 mA	234m	10 nm-rad	27 (18 ID)
ALS	1.9 GeV	500 mA	199m	2.0 nm-rad	46 (17 ID)
CHESS	6.0 GeV	200 mA	768m	27 nm-rad	8 (8 ID)
CLS	2.9 GeV	250 mA	170m	18.1 nm-rad	20 (13 ID)
CAMD	1.3 GeV	200 mA	55m	200 nm-rad	15 (3 ID)

Most important: Energy, emittance, and does it have a beamline for what I want to do?
*LCLS – X-ray free electron laser accelerator, so parameter don't easily correlate

Why choose a particular facility?

Considerations for your experiment

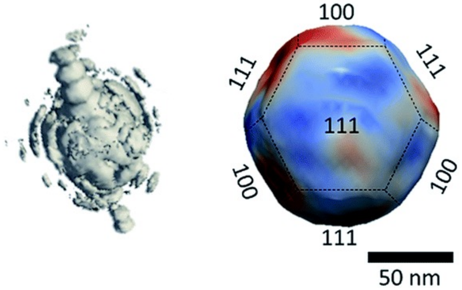
Energy range of X-rays

Higher energy storage rings generate "harder" X-rays
Penetration, complex environments, in-situ/operando

Lower energy rings
Light elements and electronic and magnetic sensitivity

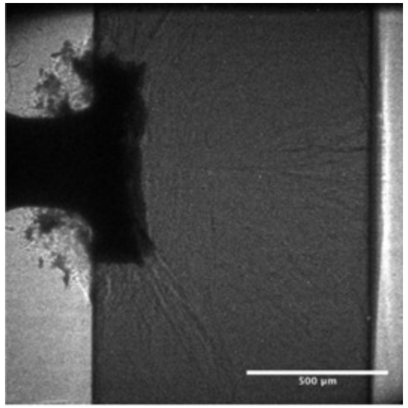
Brightness

Enables smaller focal spots and coherence-based measurements



Timing structure

Pulse structure suitable if doing ultra-fast experiments
Pump-probe and high-speed imaging



Specialized capabilities

Unique measurements
Beam polarization, magnetic field, stress/strain equipment, furnaces, laser heating, gas handling, etc.

Ancillary labs capabilities
Electrochemistry, high pressure, etc.

Location

Similar capabilities for some techniques (e.g. XAS, SAXS)

Easier to transport your own equipment

Types of synchrotron X-ray methods

Scattering and diffraction

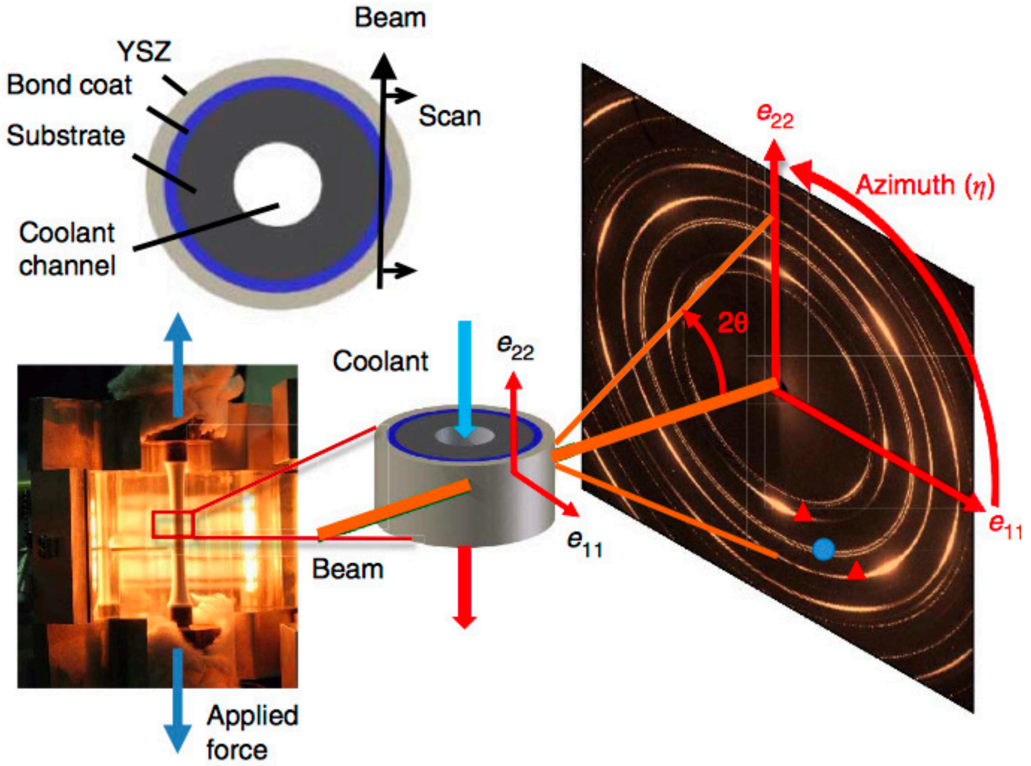
- Very high resolution
- Penetration into sample can be tuned by the incidence angle
- Tunable wavelength: anomalous scattering (element specific)
- High energy is penetrating
- Dynamical scattering
- Small-angle scattering
- Magnetic scattering

Spectroscopy

- Penetration into sample can be tuned by the incidence angle
- Fluorescence
- X-ray absorption fine structure
- Inelastic scattering
- Photoemission

Micro-scopy and imaging

Time-resolved measurements



Technology Implications
Accurate lifespan estimates of materials, wider adoption of thermal barrier coatings, increased fuel and energy efficiency for autos, airplanes, boats, and energy generation facilities. For example, 1% increase in operating temperature at a single electric generation facility can save up to $20 million a year.

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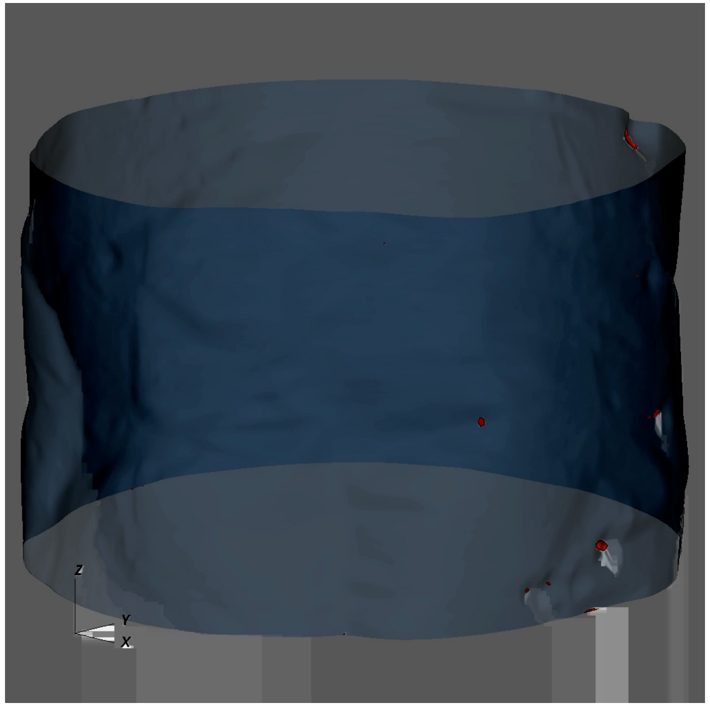
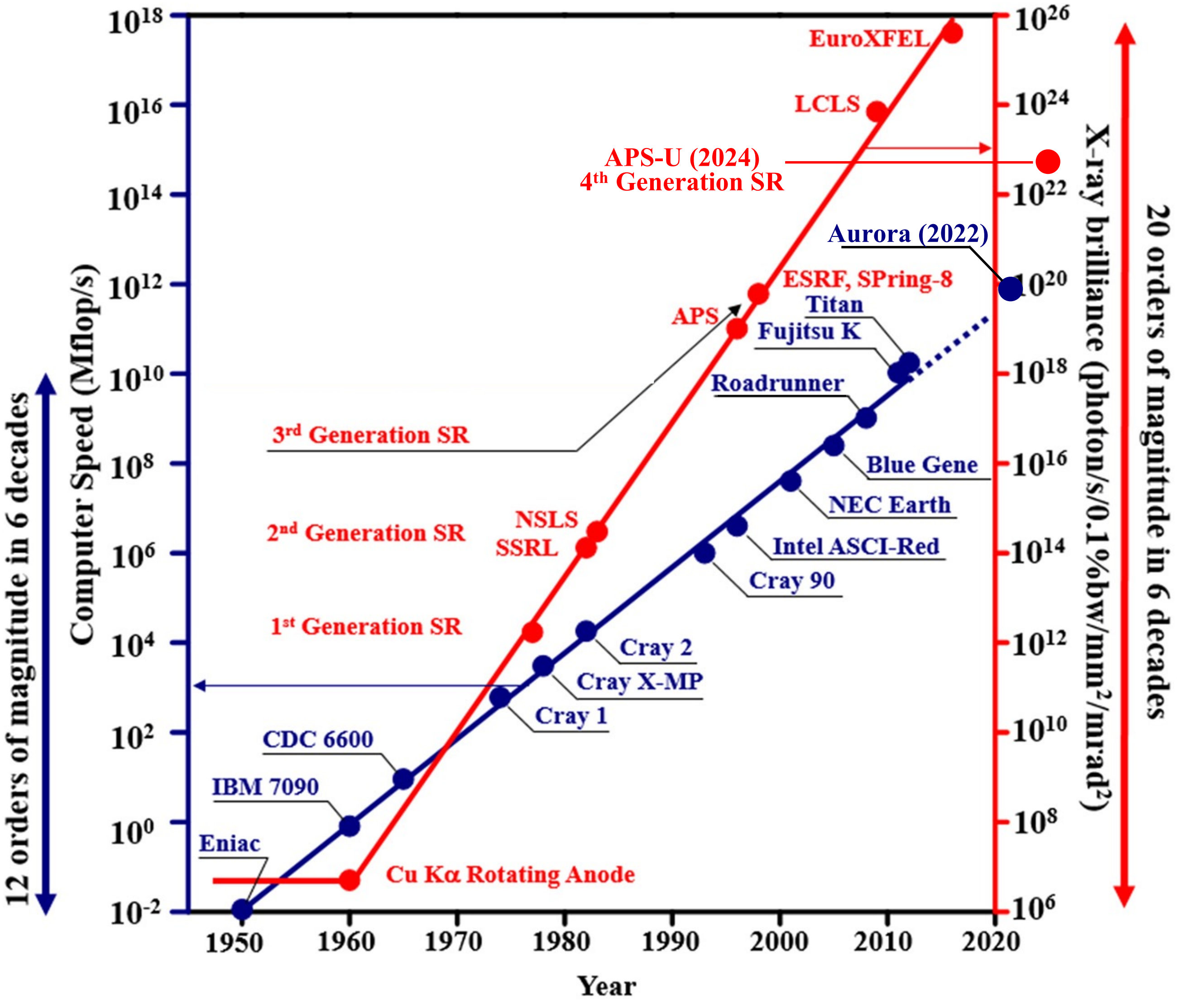
Time-resolved measure ments



Growth of Al-rich dendrite in Al-Cu alloy
Cooling rate 1K/min from 550 K
3D tomographic dataset in 1.6 s

J. W. Gibbs, K. A. Mohan, E. B. Gulsoy, A. J. Shahani, X. Xiao, C. A. Bouman, M. De Graef & P. W. Voorhees, "The Three-Dimensional Morphology of Growing Dendrites," Sci. Rep. 5, 11824 (03 July 2015).| DOI: 10.1038/srep11824

Moore’s Law for X-ray source brightness



Storage rings and free-electron lasers

Storage rings

Near continuous sources with high average brightness, wide tunable energy range, and high stability enable:

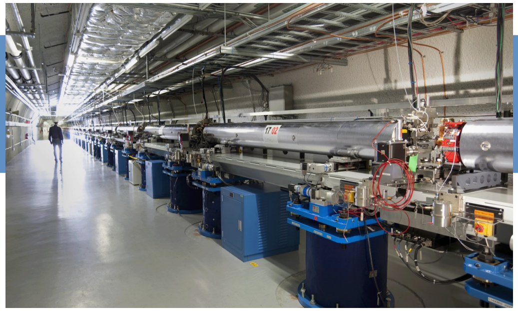
Imaging and spatially resolved spectroscopies of complex systems and processes

Balanced flux on sample to follow processes (interact but does not destroy)

Study of systems evolving on hierarchical time and length scales

Probing intrinsic atomic fluctuations with un-clocked correlation spectroscopies

Diverse, highly optimized, multiplexed end stations solving critical problems for a wide range of scientific and technological communities and numerous user groups



Free-electron lasers

Pulsed sources with ultra-high peak and average brightness with full spatial coherence enable:

Resolving ultrafast processes critical for emergent properties, excited-state transient phenomena, bond breaking and formation

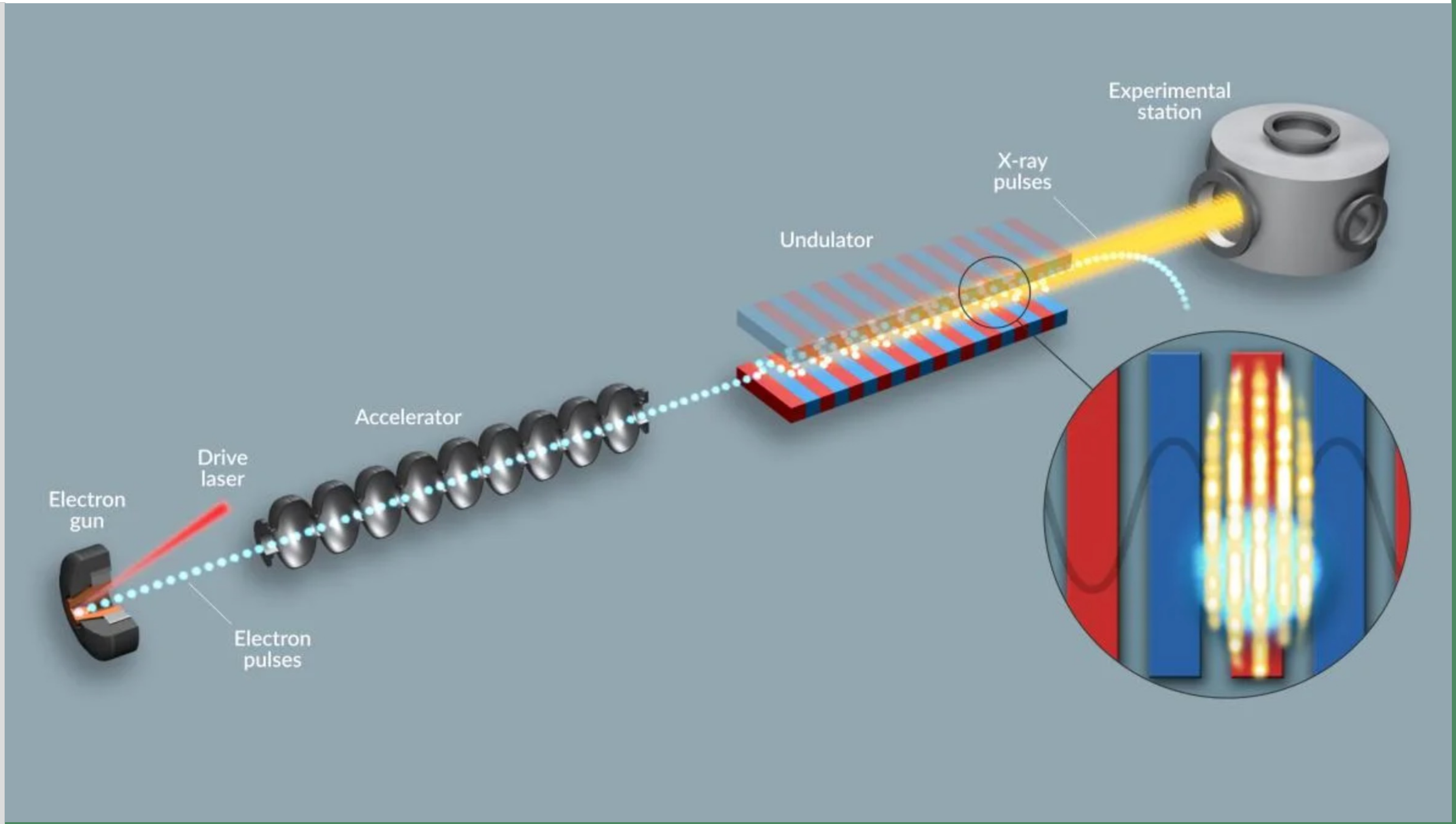
Development and application of non-linear X-ray techniques

A small number of end stations addressing carefully selected, high-profile problems

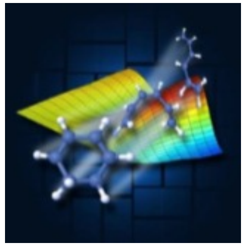
Near-instantaneous snapshots of processes in isolated areas (diffract before destroy)

XFELs: Coherent X-rays from micro-bunched electron beams

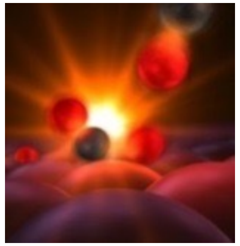
1. Microbunching starting out from noise: SASE. Strong X-ray electron interaction is key
2. X-ray pulse length < electron bunch length. Transverse coherence, with spiky time structure
3. A single temporal spike and longitudinal coherence can be provided via advanced modes of XFEL operation



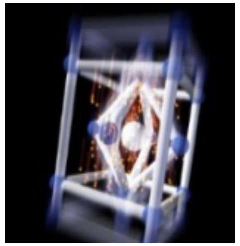
XFEL science is still in its infancy, with the next generation of sources set to further transform the field



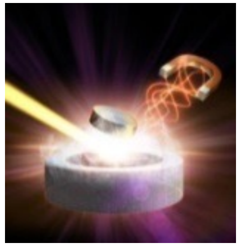
Chemical dynamics
Reaction dynamics, charge transfer, molecular photo-catalysts, natural and artificial photosynthesis



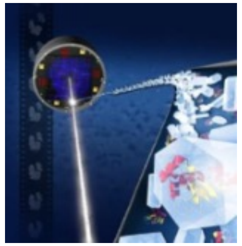
Catalysis
Homogeneous and heterogeneous catalysis, interfacial and geo/environ-mental chemistry



Materials Physics
Heterogeneity, spontaneous fluctuations, nonequilibrium dynamics, extreme environments



Quantum Materials
Emergent phenomena and collective excitations



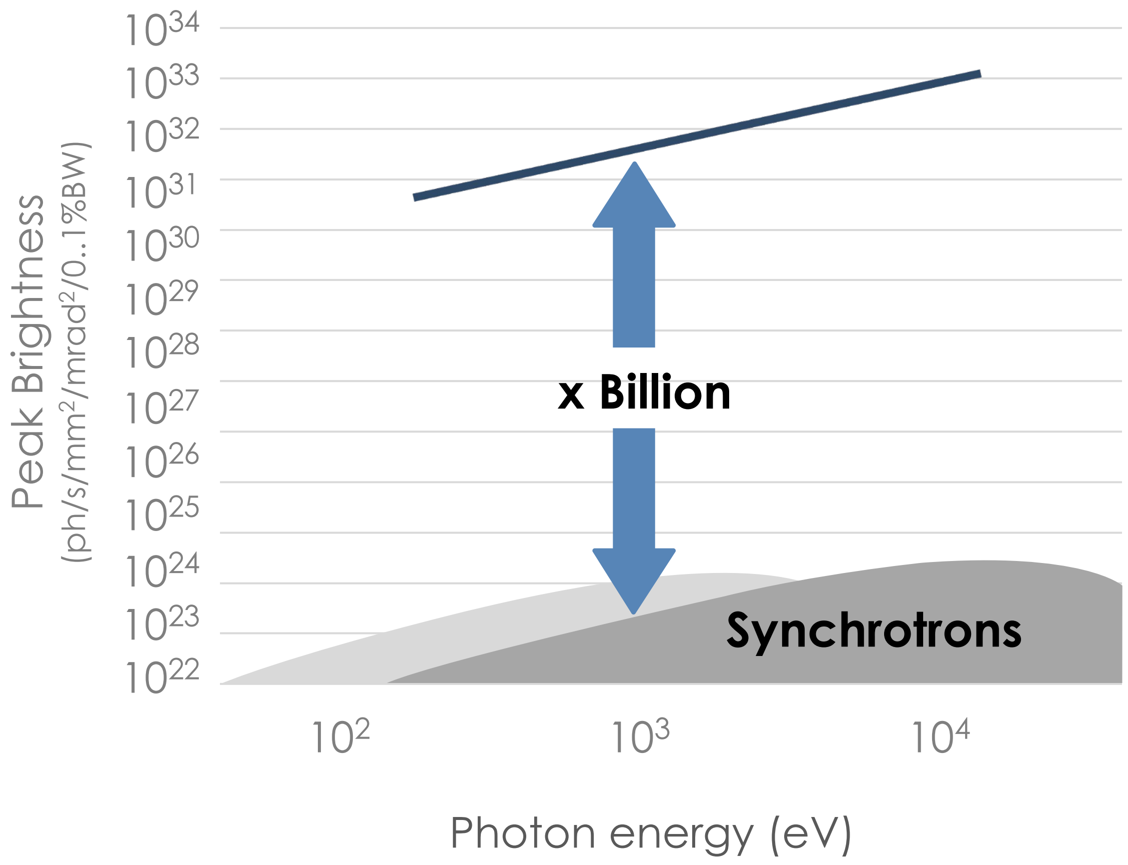
Biological Function and Structural Dynamics
Dynamics in physiological environments

Capabilities

- Transformative leap in coherent hard X-ray power (spatial and temporal)
  - >1000-fold increase in average spectral brightness
- State-of-the-art instrument suite
- Tunable, controllable beams
  - Femtosecond
  - Hard X-ray
  - Programmable time structure
  - Up to 1 MHz CW

XFELs are designed to be game-changing scientific tools

(10^9 times brighter than synchrotron sources)



LCLS, US
2009

SACLA, Japan
2011

PAL-XFEL, Korea
2017

SwissFEL, Switzerland
2017

European XFEL, Germany
2017

SHINE, China
Under construction (2026-27)

Soft X-ray FEL facilities:

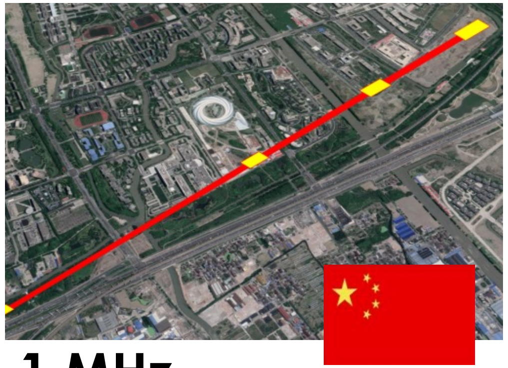
- FLASH (Germany)
- FERMI (Italy)
- SXFEL (China)

OAK RIDGE National Laboratory

XFELs are now entering their second generation

MHz rates with average power >1000x times a synchrotron source

1 MHz
LCLS, USA
X-ray sources: 2



1 MHz
SHINE, China, 2026-27
X-ray sources: 3

100 Hz
SwissFEL, Switzerland
X-ray sources: 2

60 Hz
SACLA, Japan
X-ray sources: 2

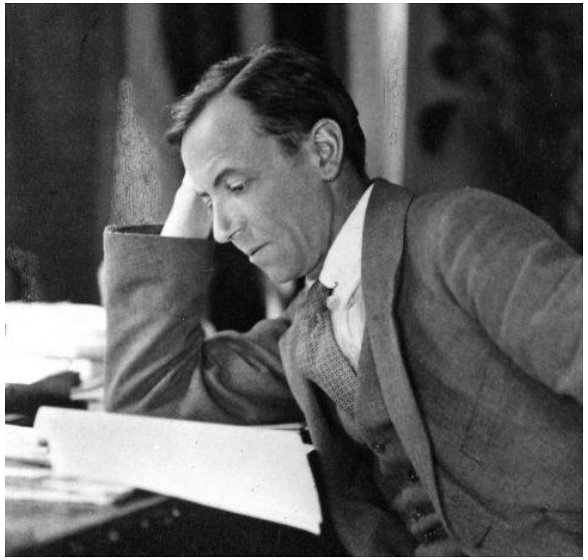
60 Hz
PAL-FEL, Korea
X-ray sources: 2

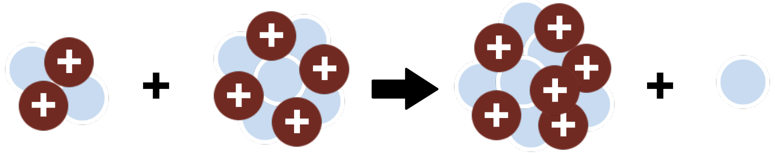
27 kHz avg.
(10 Hz / 4.5 MHz)
EuXFEL, Germany
X-ray sources: 3

Neutron user facilities

The first neutron source

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

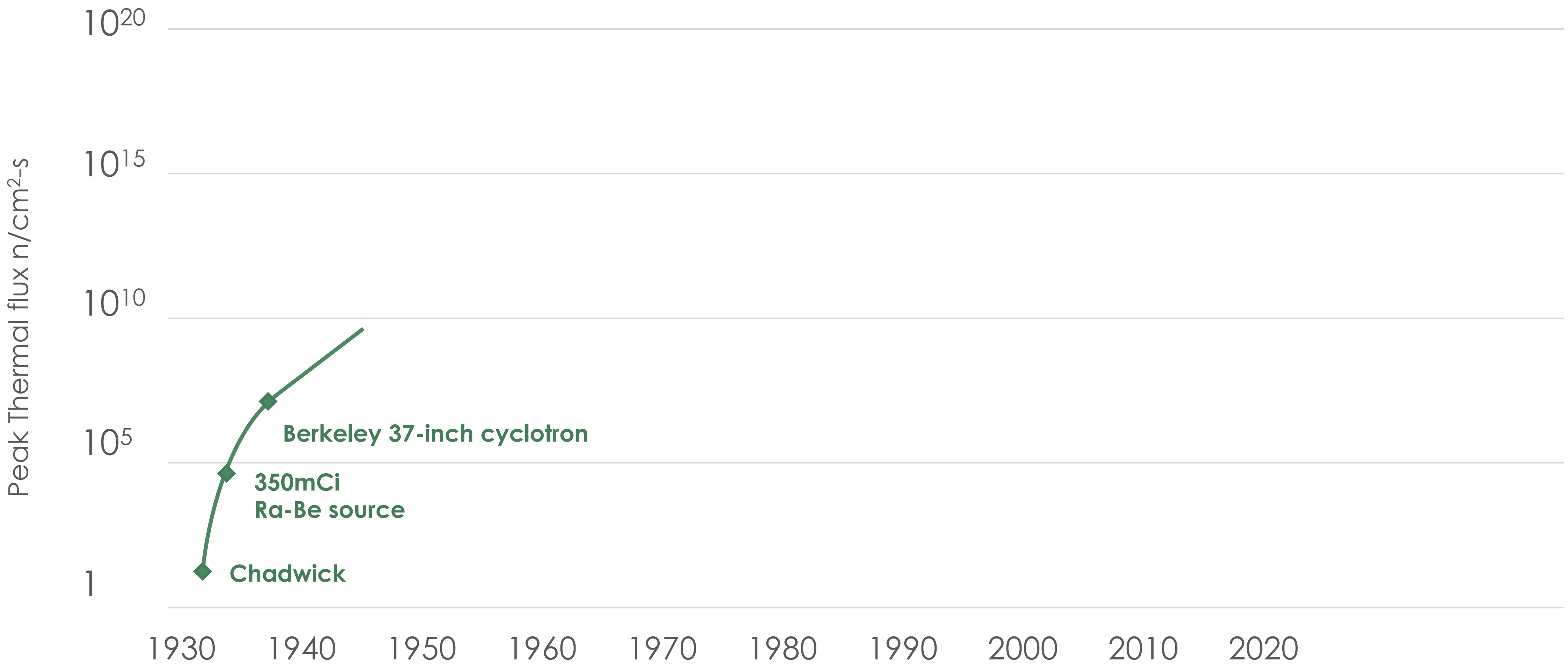




$^{4}He + {}^{9}Be \rightarrow {}^{12}C$ + **neutrons**

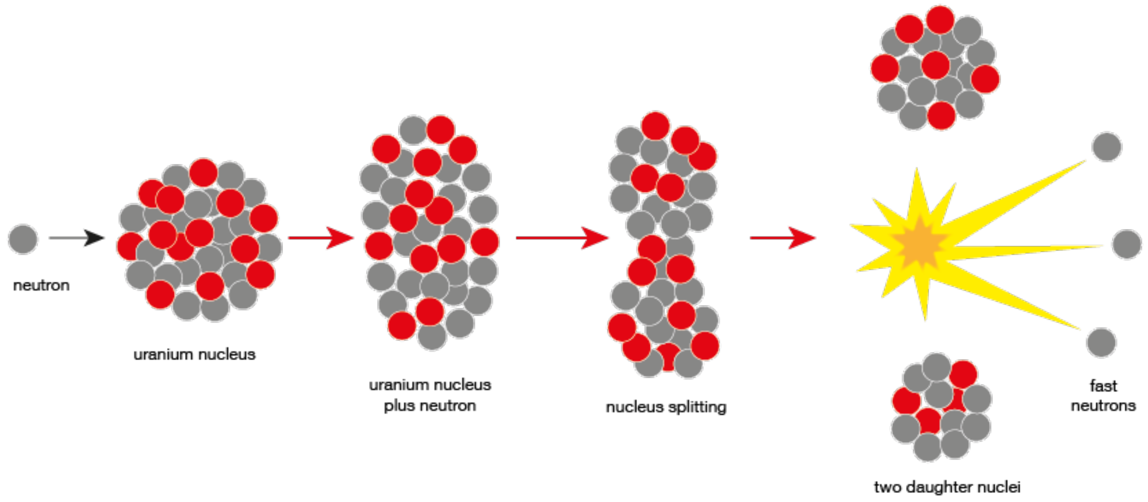
James Chadwick
Used Polonium as alpha emitter on Beryllium

Evolution of neutron sources



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

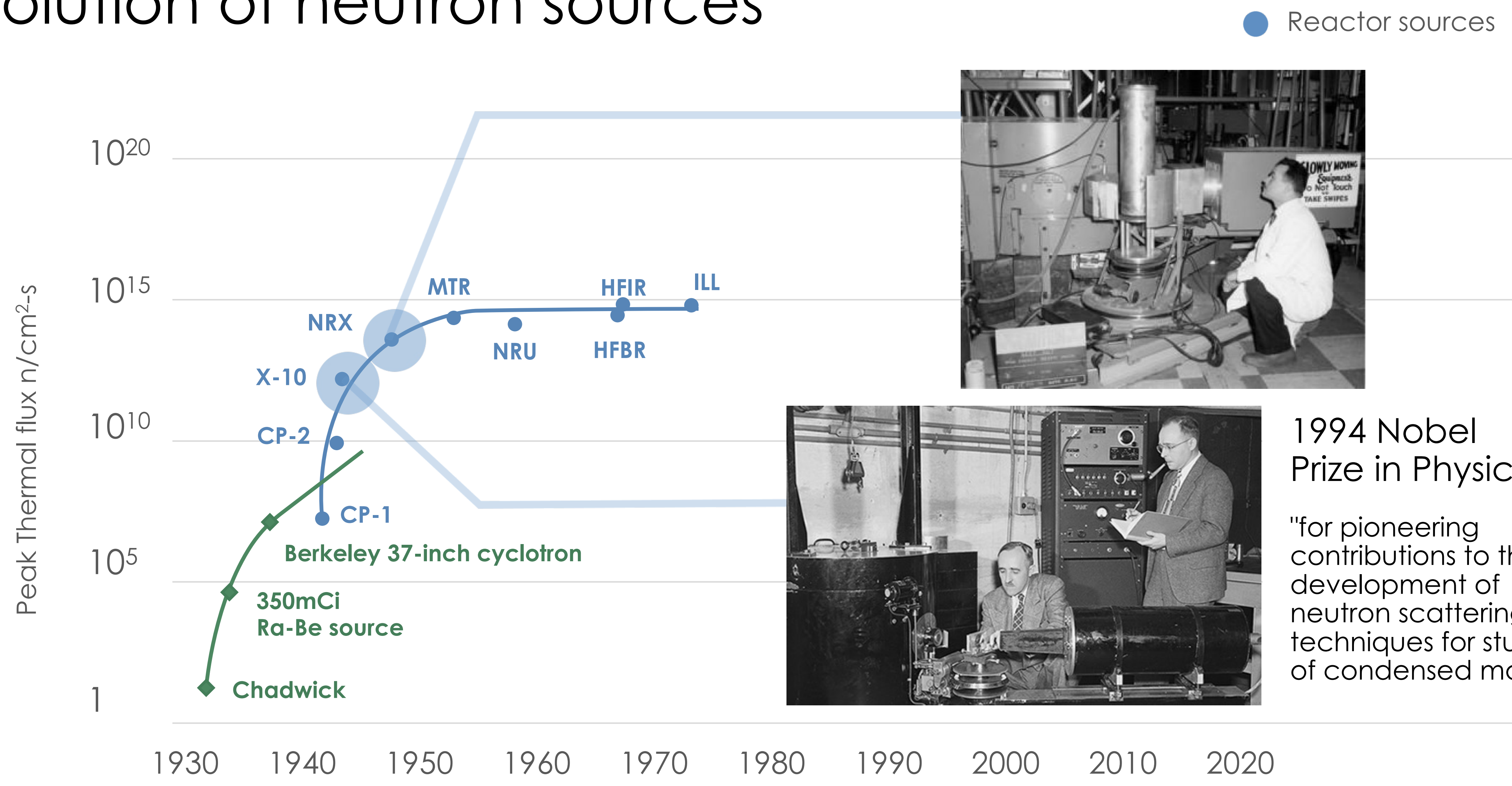
Nuclear fission



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

December 2, 1942

Evolution of neutron sources

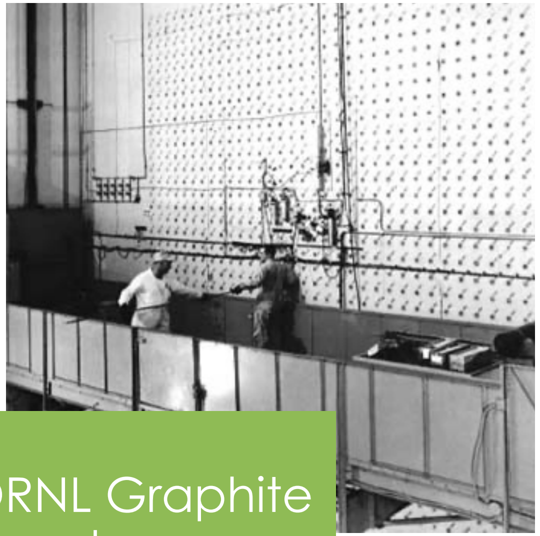


1994 Nobel Prize in Physics

"for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

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

Nuclear reactor power drives new scientific innovation



ORNL Graphite Reactor

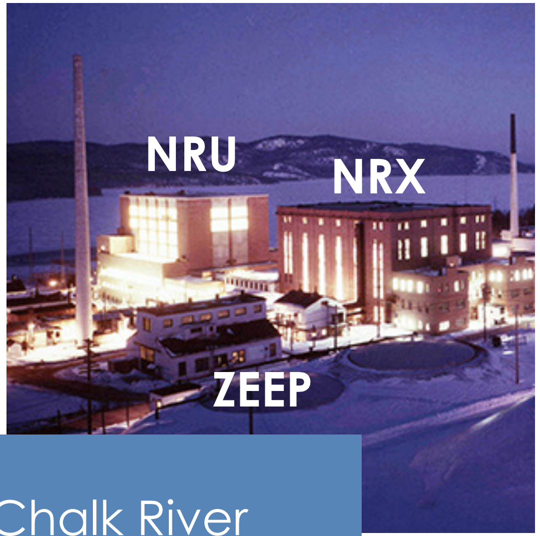
Critical on **Nov. 4, 1943**

- 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!

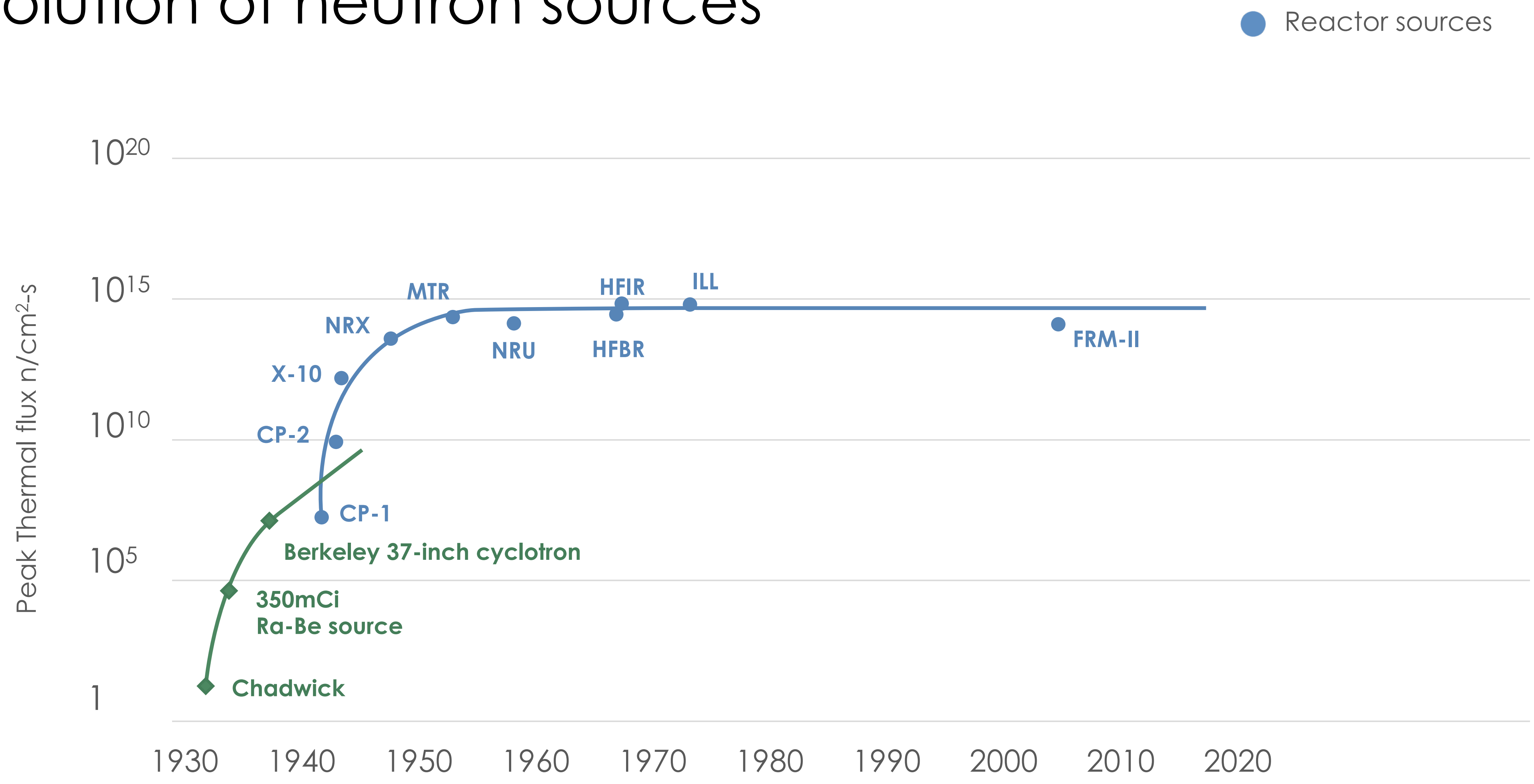


Chalk River NRU Reactor

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



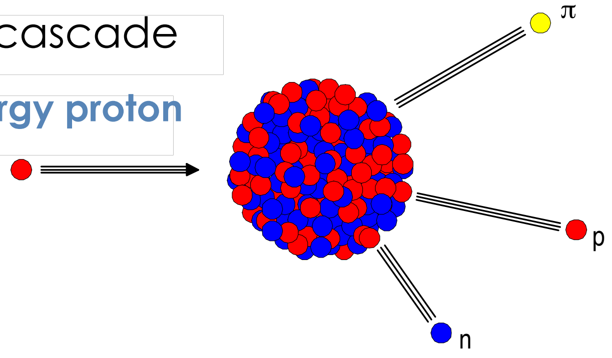
(Updated from *Neutron Scattering*, K. Sköld and D. L. Price, eds., Academic Press, 1986)

Nuclear spallation

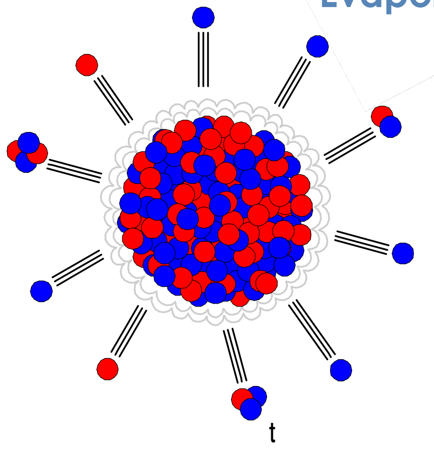
1 GeV proton in:
250 MeV becomes mass (endothermic reaction)
30 neutrons freed
⇒ 25 MeV/neutron
6x more efficient than fission

First stage:
Intranuclear cascade

High-energy proton

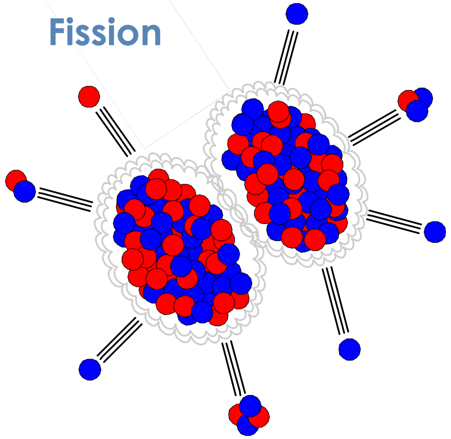


Intermediate stage:
Pre-equilibrium

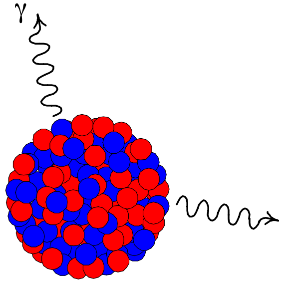


Evaporation

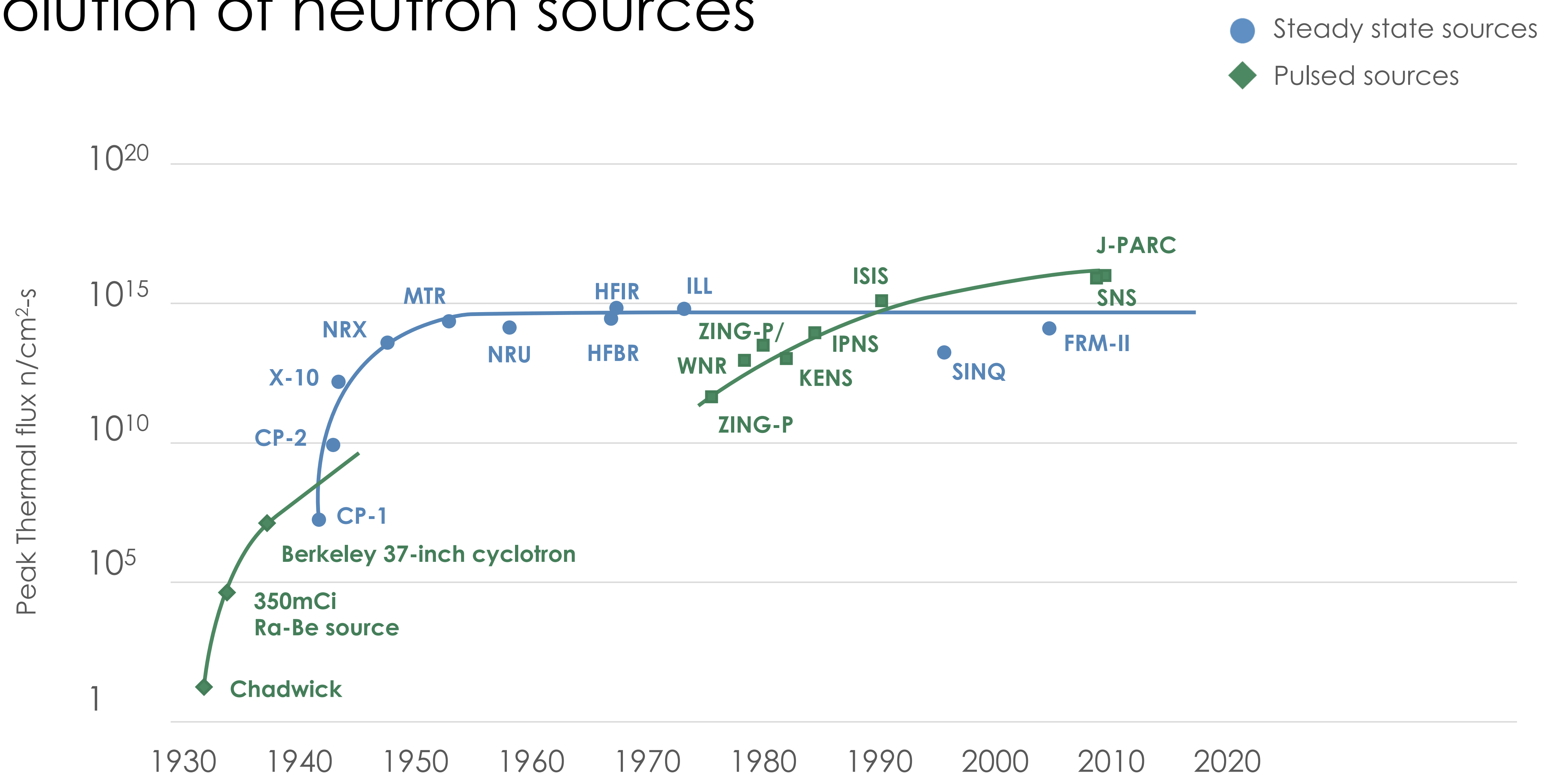
Fission



Final stage:
Residual de-excitation



Evolution of neutron sources



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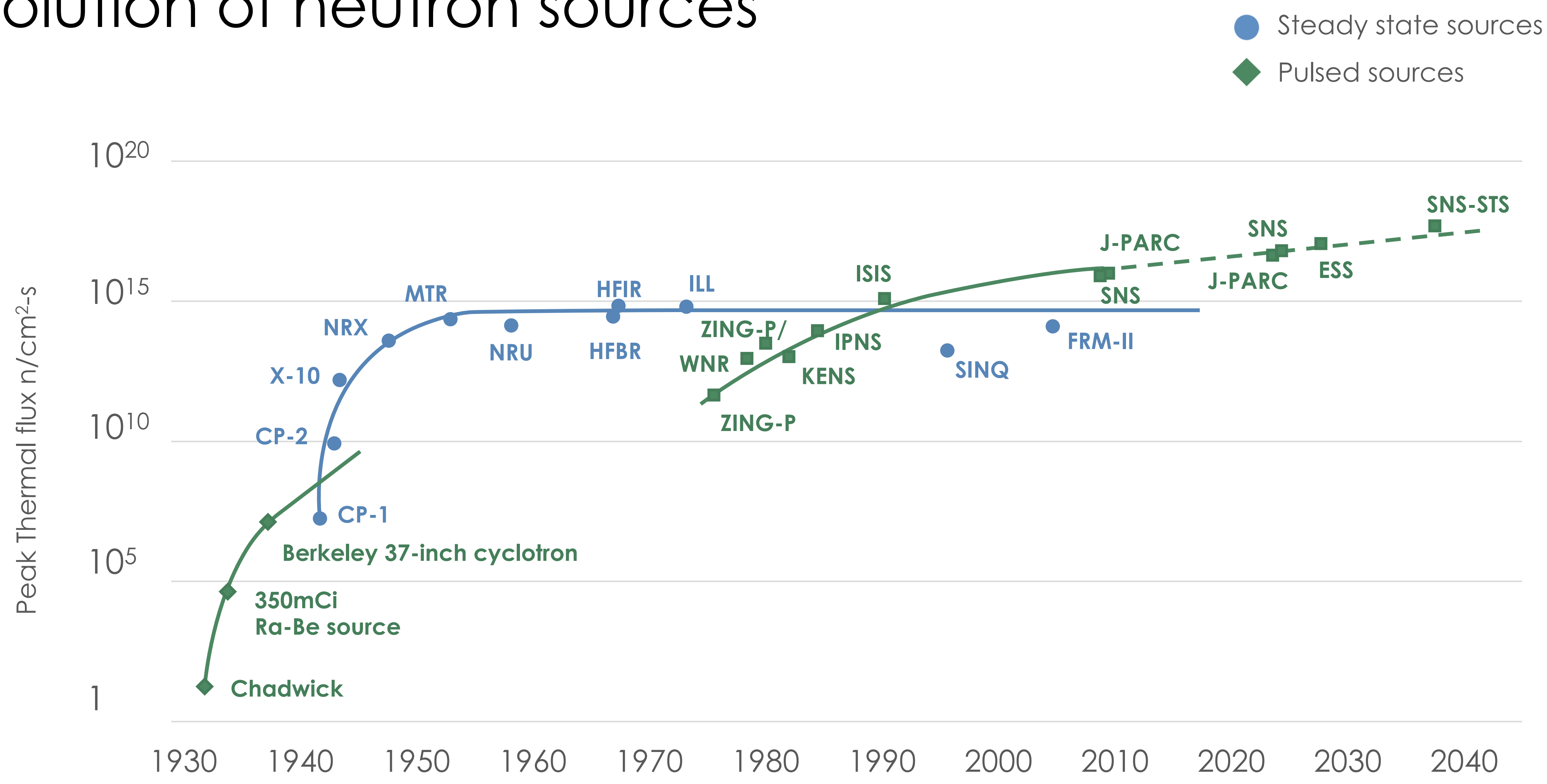
Evolution of neutron sources



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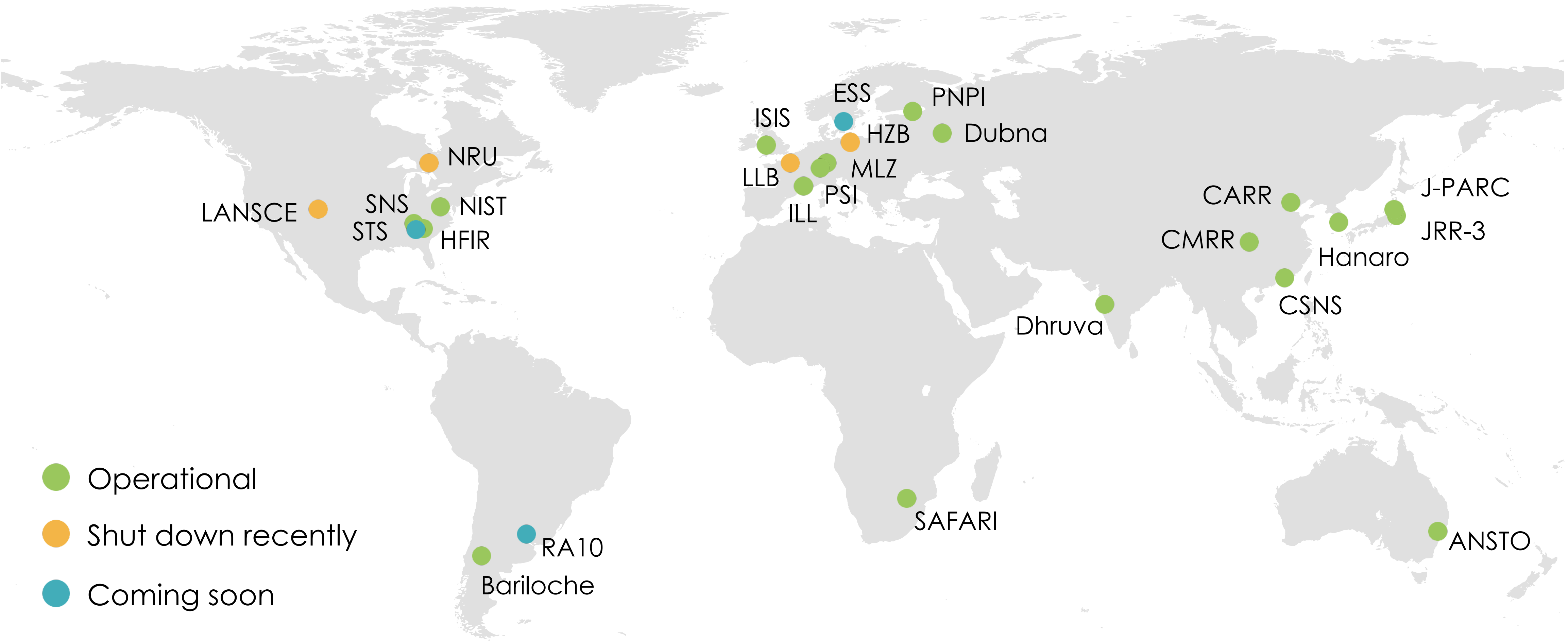
Neutron user facilities worldwide



Neutron user facilities in North America

High Flux Isotope Reactor (HFIR)

Operates at 85 MW and provides highest steady-state neutron fluxes in the world for materials research

12 instruments in user program

Spallation Neutron Source (SNS)

Most powerful pulsed neutron source in the world for materials research

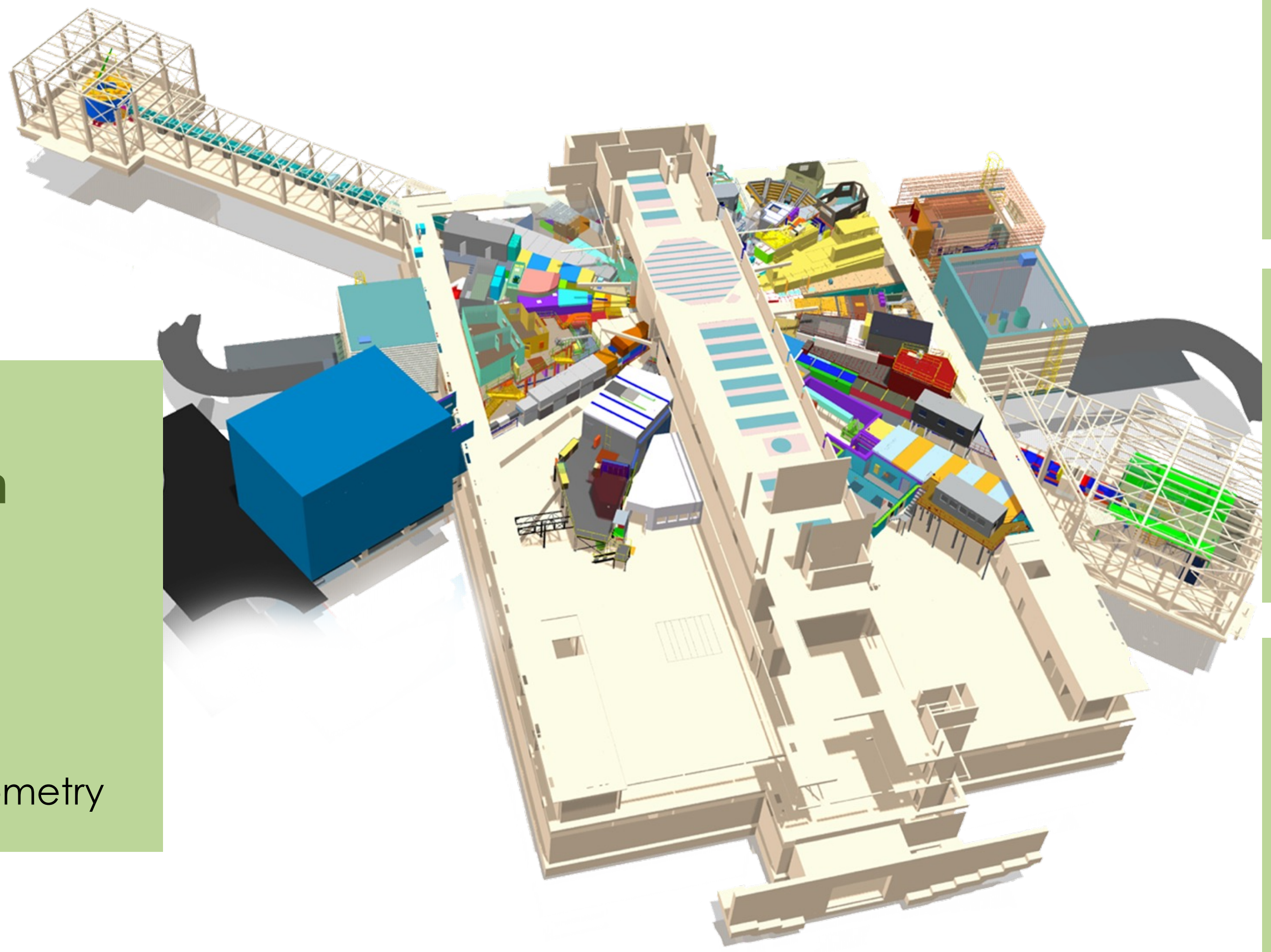
18 instruments in user program

NIST Center for Neutron Research (NCNR)

20 MW reactor in Gaithersburg, MD

13 instruments in user program

Spallation Neutron Source



18 instruments in user program

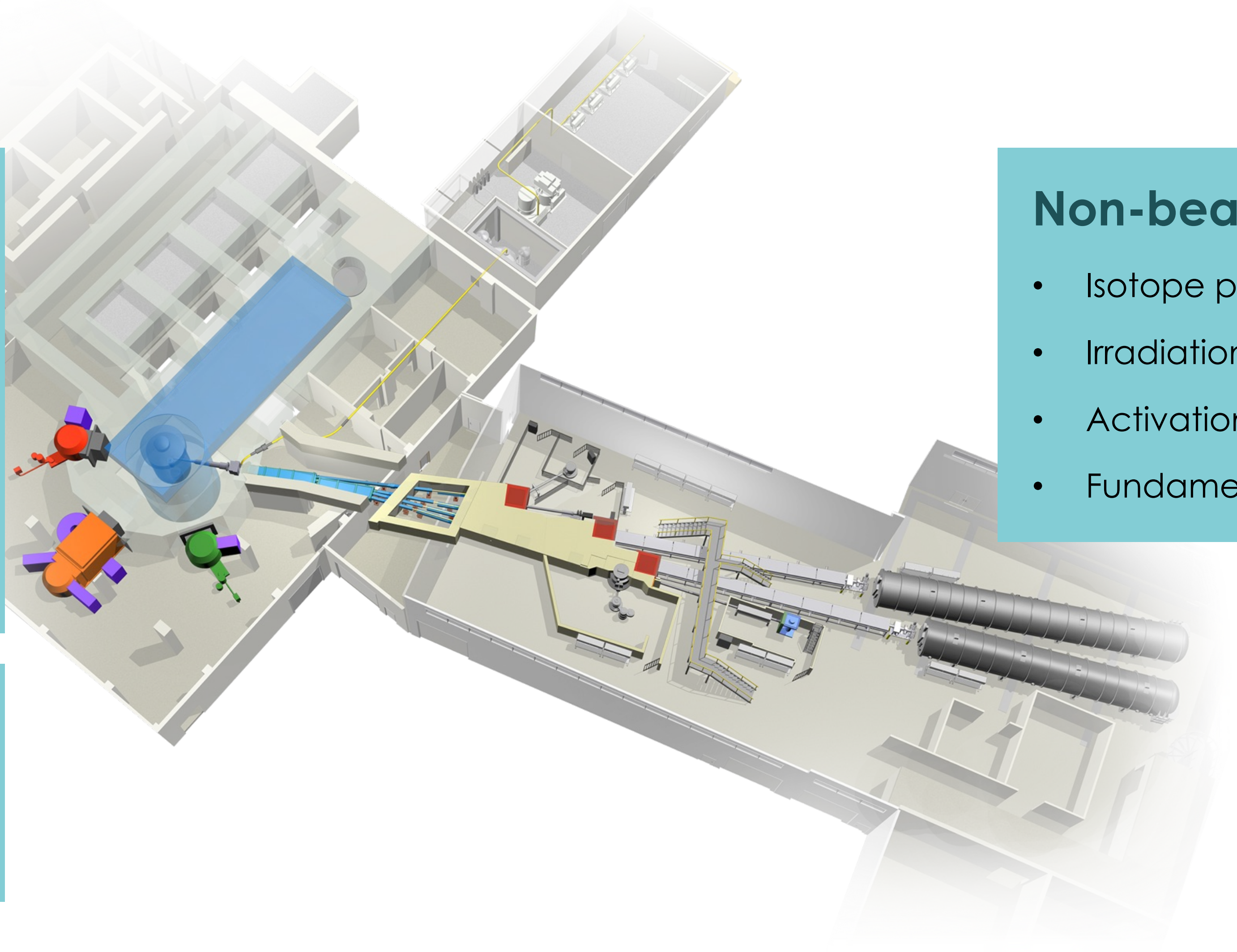
- Diffraction
- Spectroscopy
- Engineering
- SANS and reflectrometry

1 instrument 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

Thank you!

NXS Lecture - Stephen Streiffer:
“X-ray and Neutron User Facilities”

Oak Ridge National Laboratory