The European Spallation Source

Workshop on Early Science on the NMX Macromolecular Diffractometer

August 26th 2024, Padova

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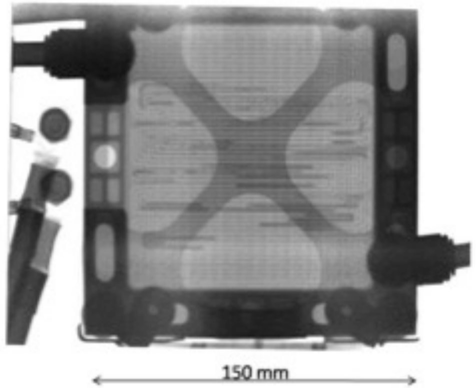
HEAD - LARGE SCALE STRUCTURES DIVISION

2024-08-26

Why Neutrons?

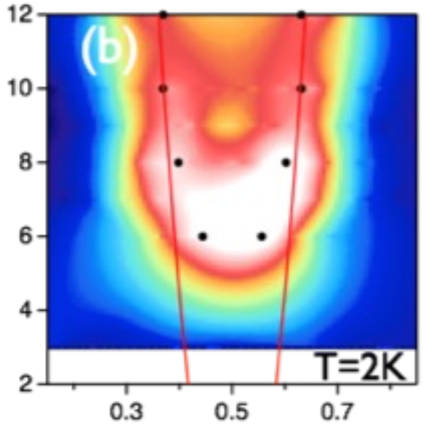
Neutrons have special properties …

Charge neutral
Deeply penetrating



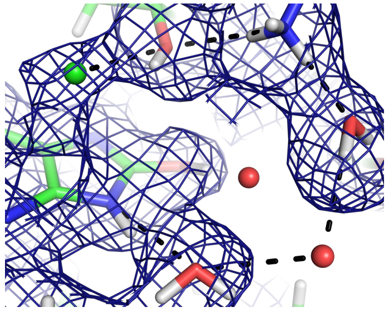
Hydrogen and water distribution in fuel cells

Magnetic moment (spin)
Probe of magnetism



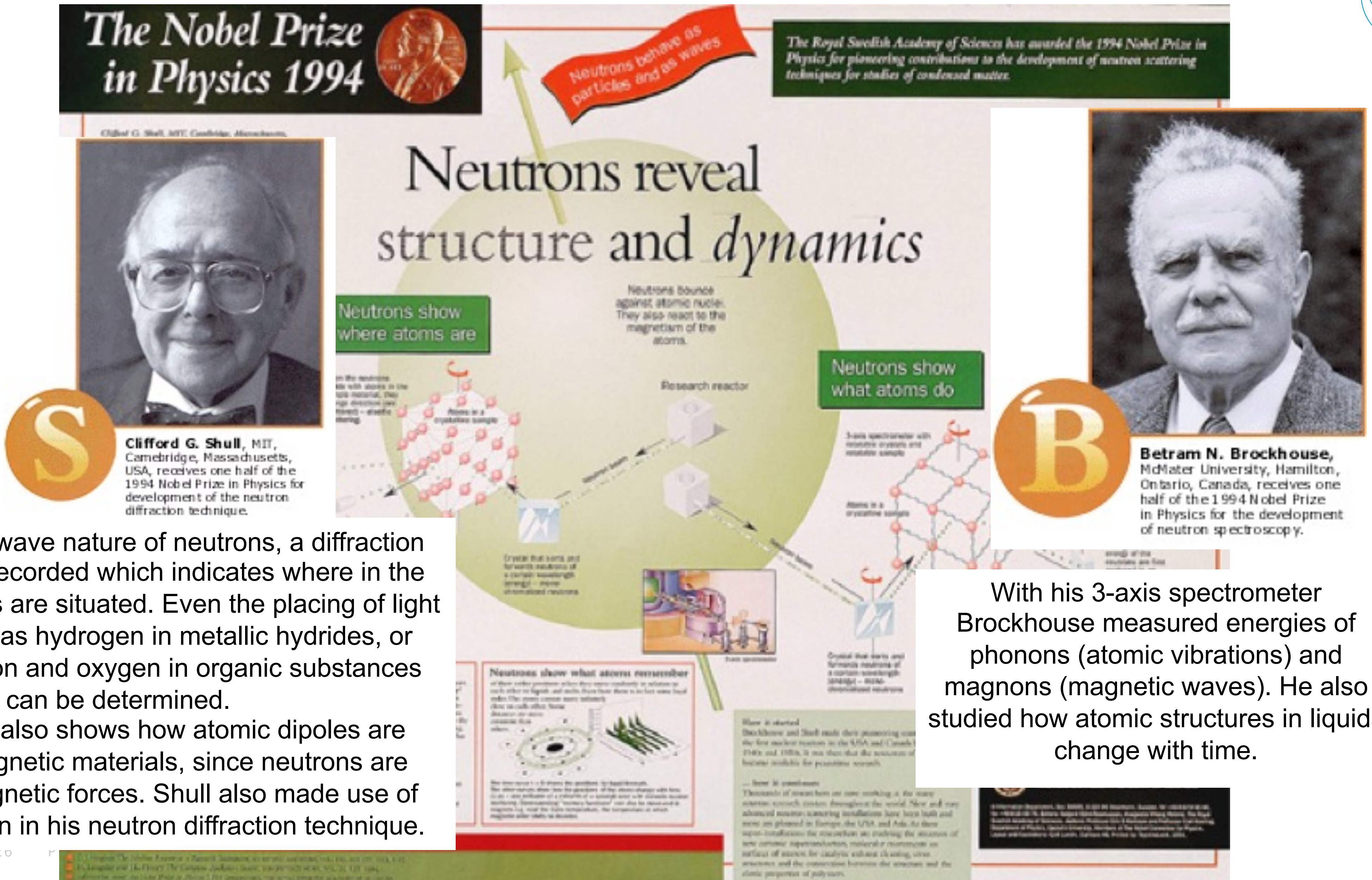
Understanding supercondutors

Nuclear scattering
Sensitive to light elements and isotopes



Understanding drug binding and enzyme action

Geometry of Motion



Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. Even the placing of light elements such as hydrogen in metallic hydrides, or hydrogen, carbon and oxygen in organic substances can be determined.

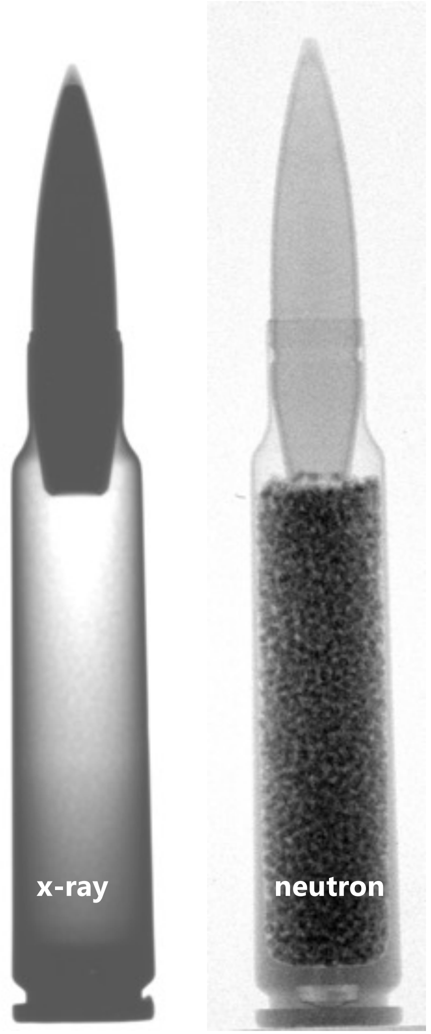
The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.

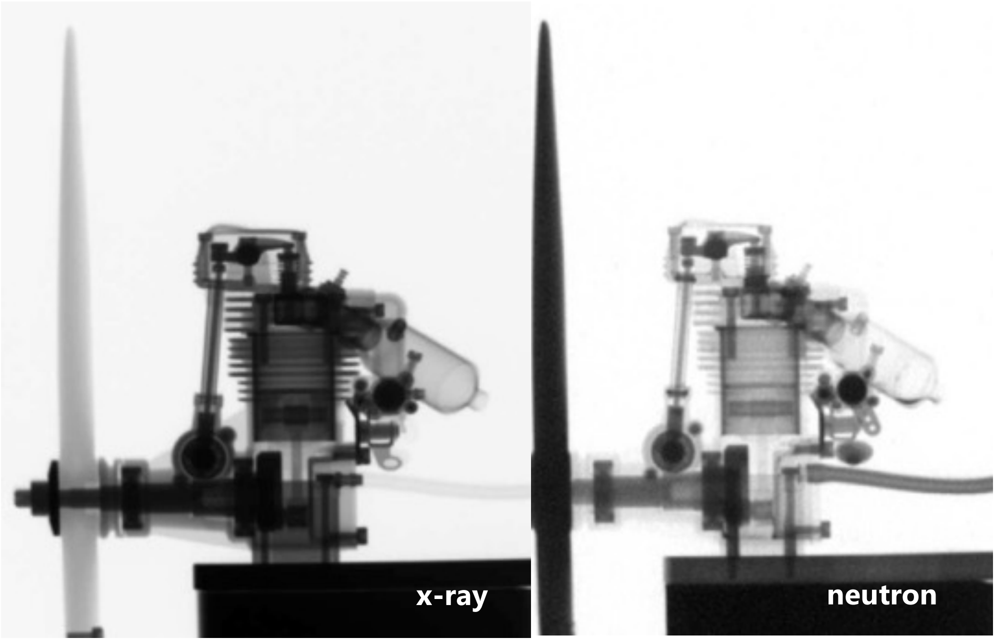
With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structures in liquids change with time.

X-Rays and Neutrons

Different views of the same thing

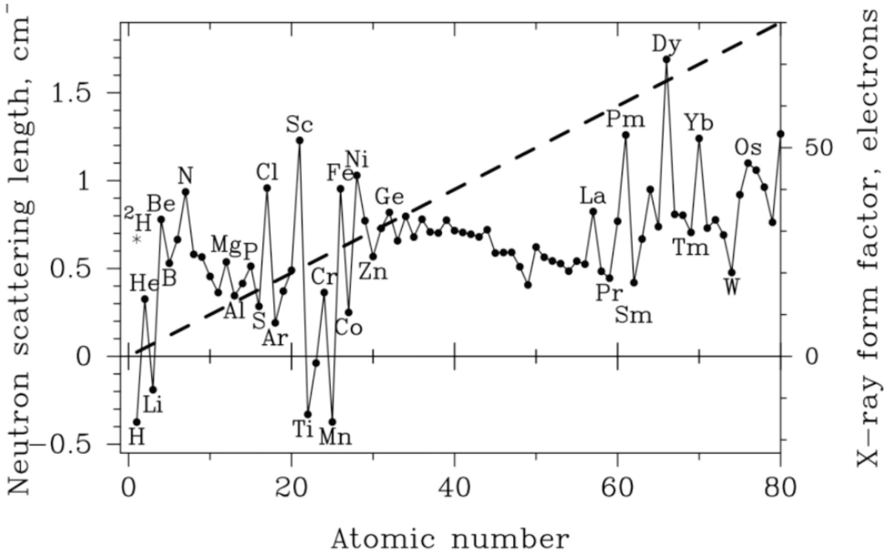
Courtesy of the NIAG group, PSI, Switzerland.

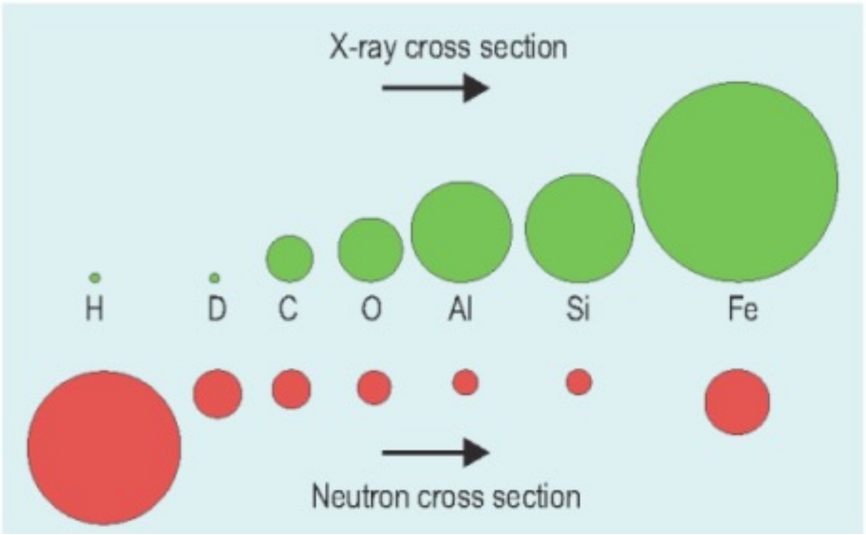




Due to the different interaction and cross sections, neutrons and x-rays provide complementary information

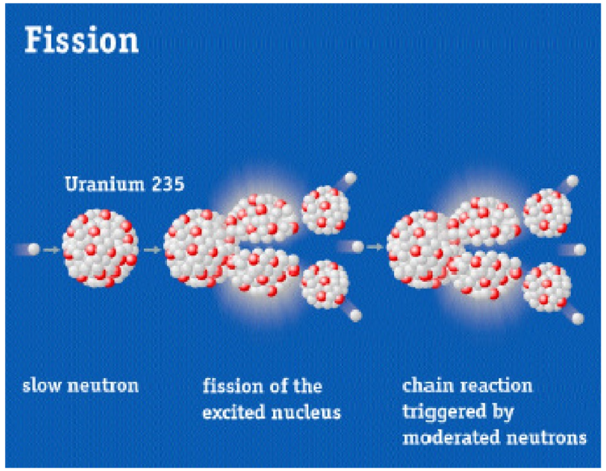
X-Rays and Neutrons





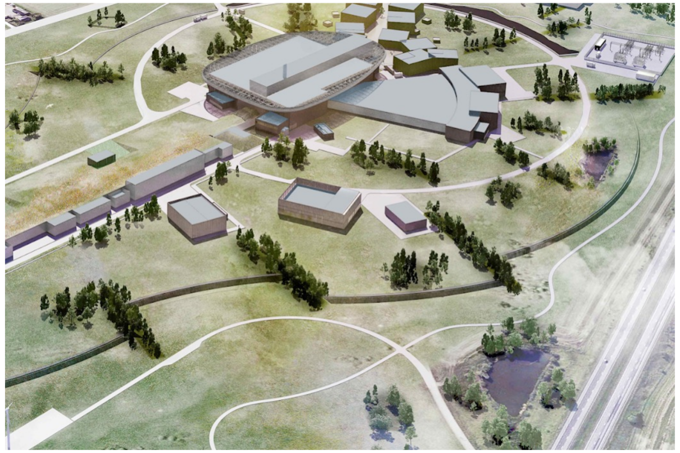
	X-Ray	Neutron
Mass	None	1.674928×10^{-27} kg (1839 electrons)
Spin	1	1/2
Magnetic Moment	None	-1.9130427 μ_n
Energy	10 eV – 100 keV	0.1 meV – 0.5 eV
Wavelength	0.01 nm to 100 nm	0.01 nm to 3 nm
Source brightness	$10^6 - 10^{20}$ (photons/mm^2/s/mrad/0.1% bandwidth)	$10^{10} - 10^{14}$ (neutrons/cm2/s/sr/Å)

Production of neutrons



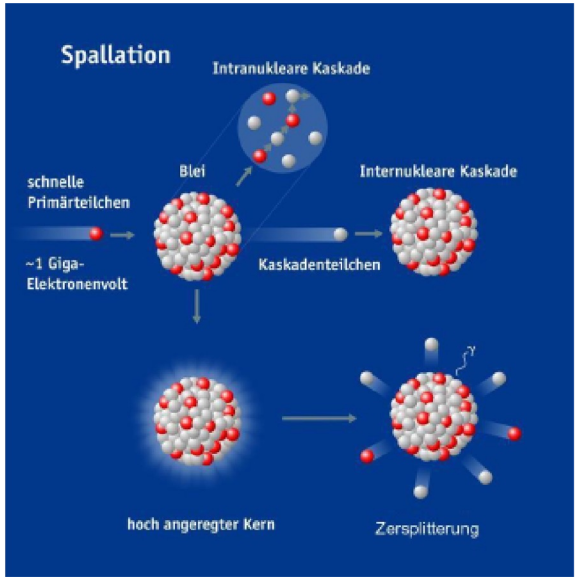
Fission of uranium
in nuclear reactor

2-3 neutrons per process

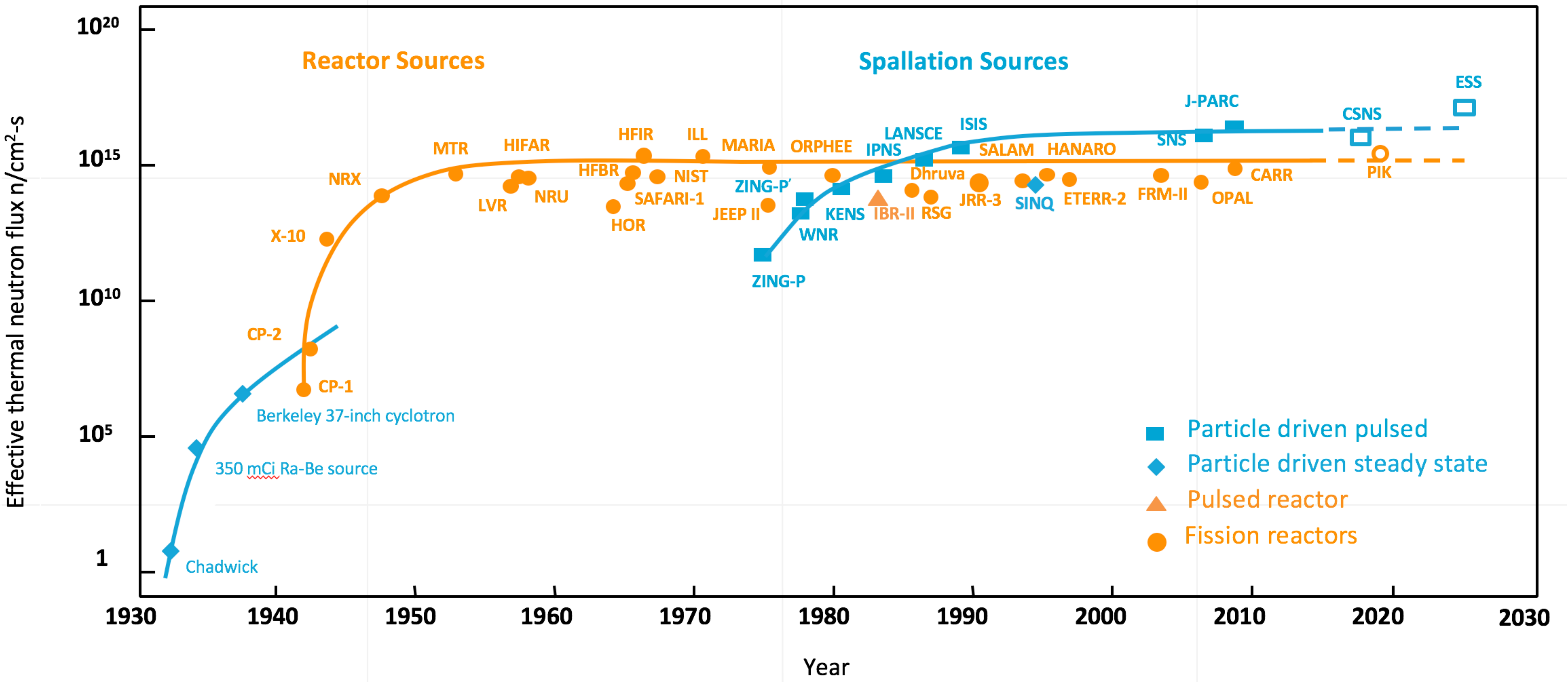


Spallation on target
using proton accelerator

30+ neutrons per process



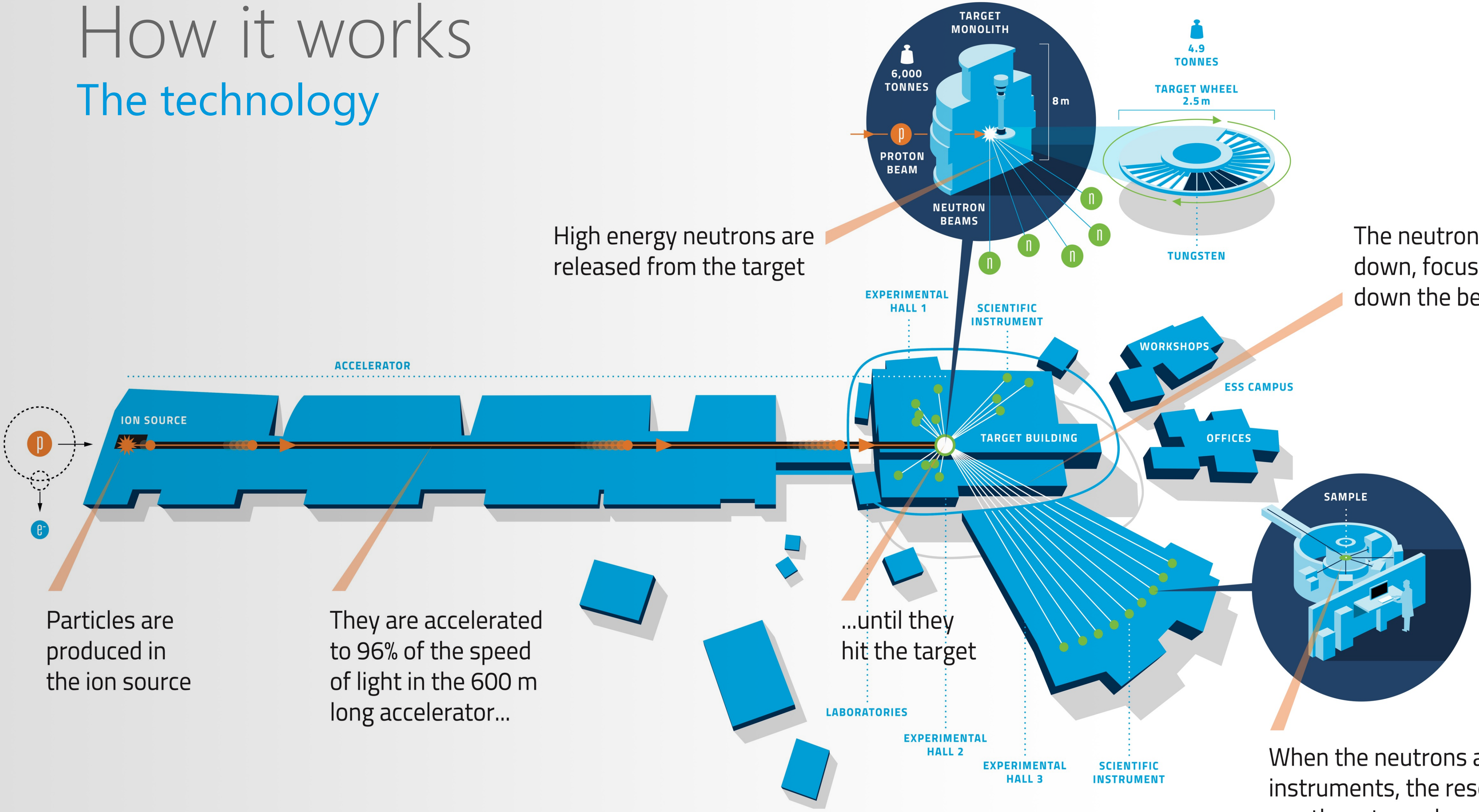
Neutron Source Brightness



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

How it works

The technology



Particles are produced in the ion source

They are accelerated to 96% of the speed of light in the 600 m long accelerator...

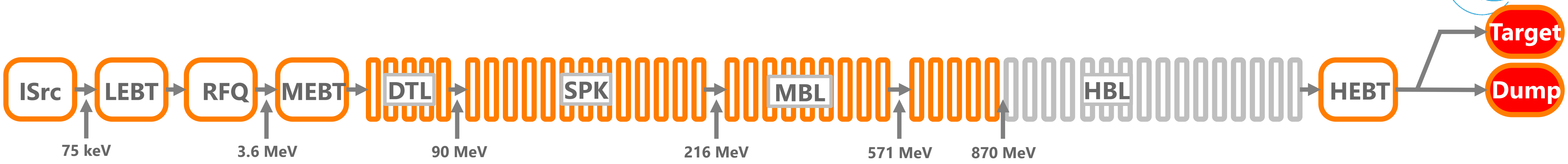
...until they hit the target

High energy neutrons are released from the target

The neutrons are slowed down, focused and sent down the beamlines

When the neutrons arrive at the instruments, the researchers can use them to explore materials down to an atomic level

High Power 5MW Proton Accelerator



The ESS accelerator was designed and is built by a collaboration of 23 institutes and universities in Europe

More then 50% of the total budget is delivered as In-kind with most systems being IK deliveries. The main exceptions are the cryo plants, the 704 MHz klystrons and modulators.

ESS accelerator division is responsible for functional requirements, coordination of work, installation including infrastructure, testing & commissioning and operation.

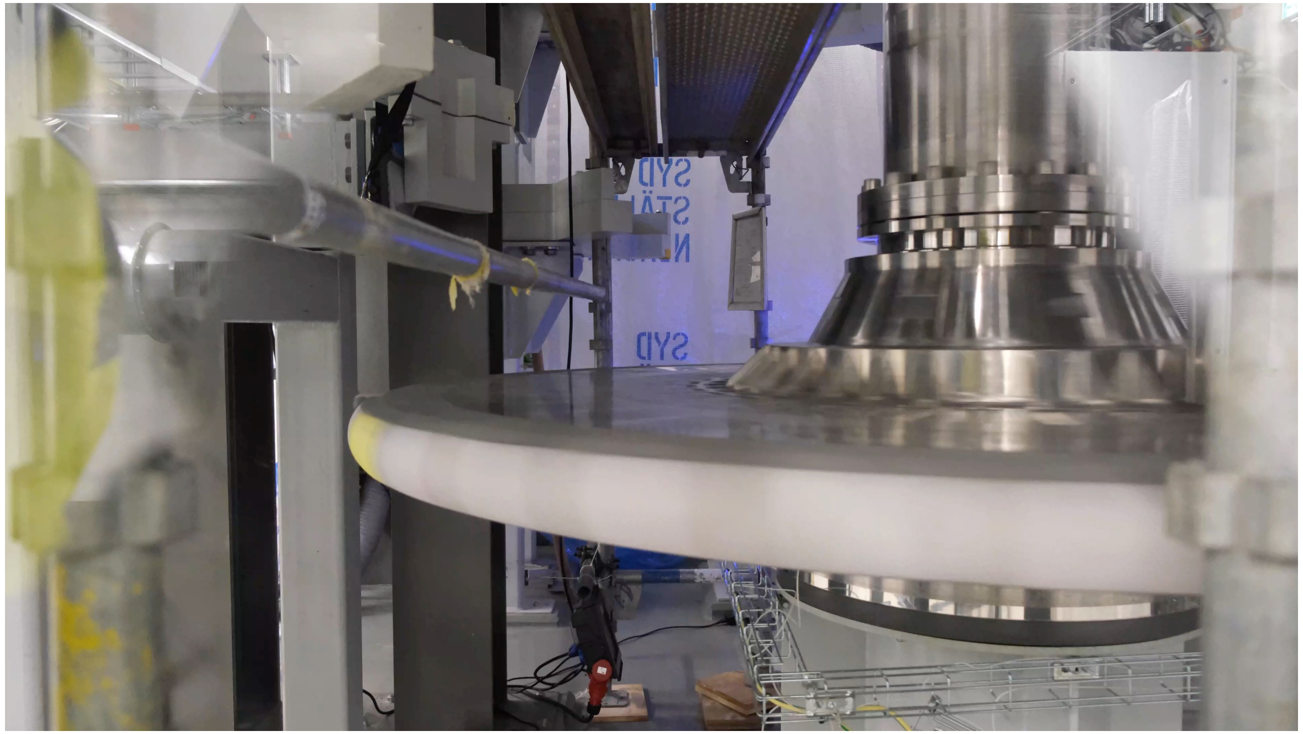
The linac shall in the full scope deliver **5 MW at 2 GeV, 14 Hz with 2.86 ms long pulses**

For Beam on Dump and Ready for Beam on target the accelerator will operate at **572 MeV able to put 1.4 MW on the target with nominal duty-cycle.** Planned with the medium beta elliptical section , but two high beta will be used to compensate for medium beta cavities needing reprocessing

For End-Of-Construction in 2027, an additional cryomodules will be installed and powered enabling operation at **2 MW, 870 MeV with nominal duty cycle**

The remaining cryomodules will be installed in the tunnel during shutdowns but not powered with RF. Control and operation of e.g. tuners and cryogenics will be available for all cryomodules.

Target Wheel

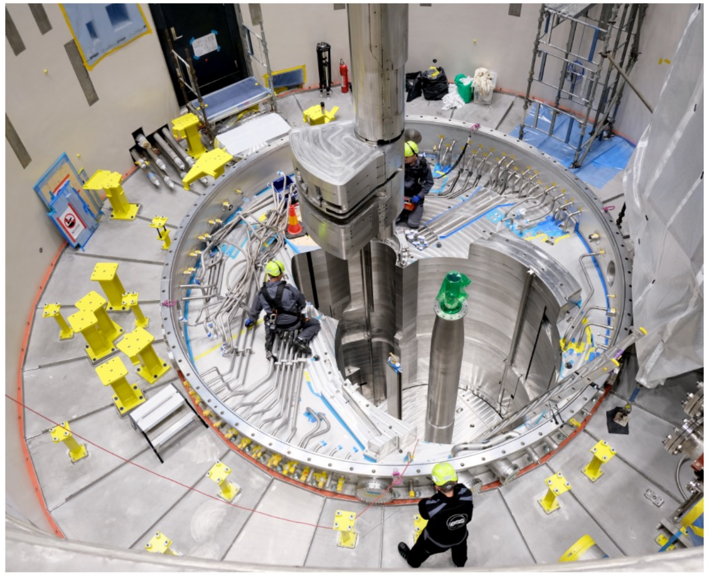


Getting the right energy

The neutrons generated must often be **moderated** to lower their energy (increase their wavelength) before they are used in scattering experiments

Moderation at reactor : water, liquid hydrogen or liquid deuterium

Moderation at spallation source : water, liquid hydrogen or solid methane

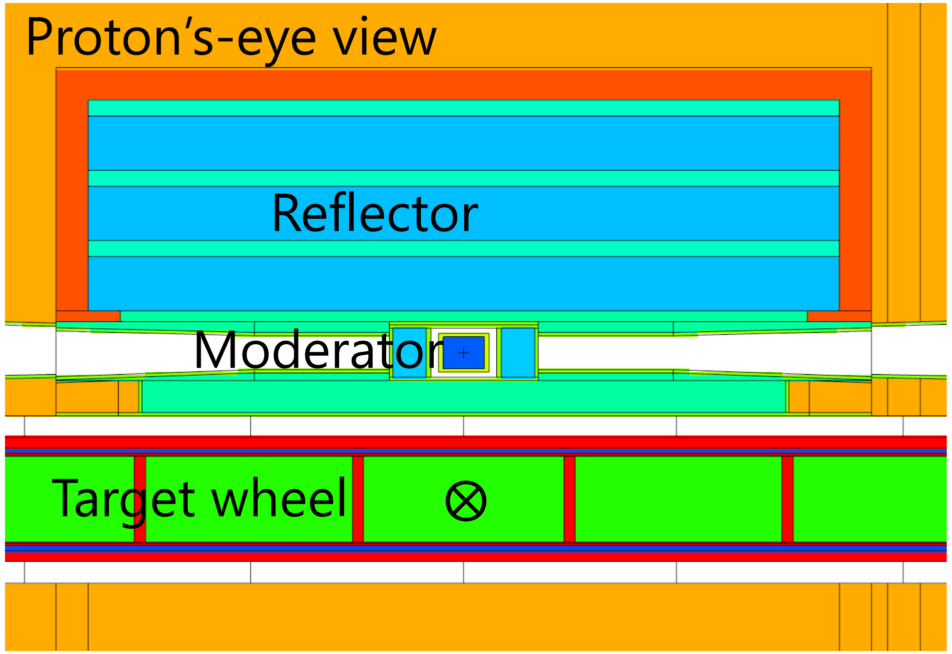


Boltzmann: $E = k_B T$

$$E = k_B T = \frac{1}{2} m v^2 = \frac{h}{2m\lambda^2}$$

De Broglie: $\lambda = \frac{h}{mv}$

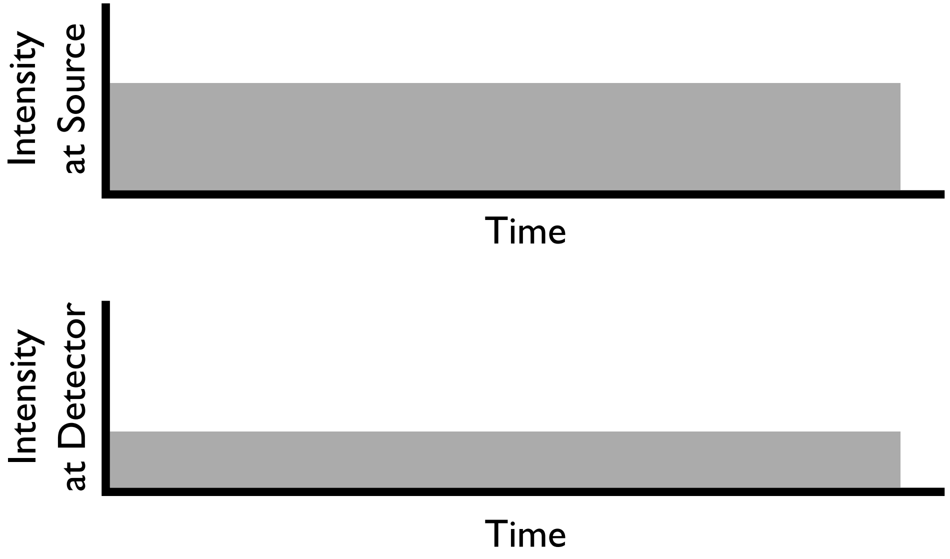
Source	Energy	Temperature	Wavelength
cold	0.1-10	1-120	30-3
thermal	5-100	60-1000	4-1
hot	100-500	1000-6000	1-0.4



Proton beam in

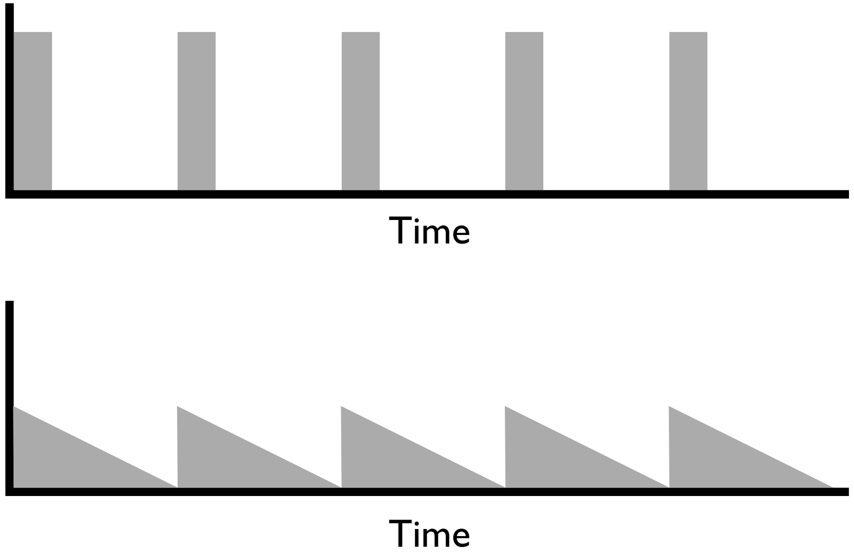
“Monochromatic” vs Time-of-Flight

Continuous Source
"Monochromatic"



Some of the neutrons all of the time

Pulsed Source
Time-of-Flight



All of the neutrons some of the time

$$Q = \frac{4\pi}{\lambda} sin\theta$$

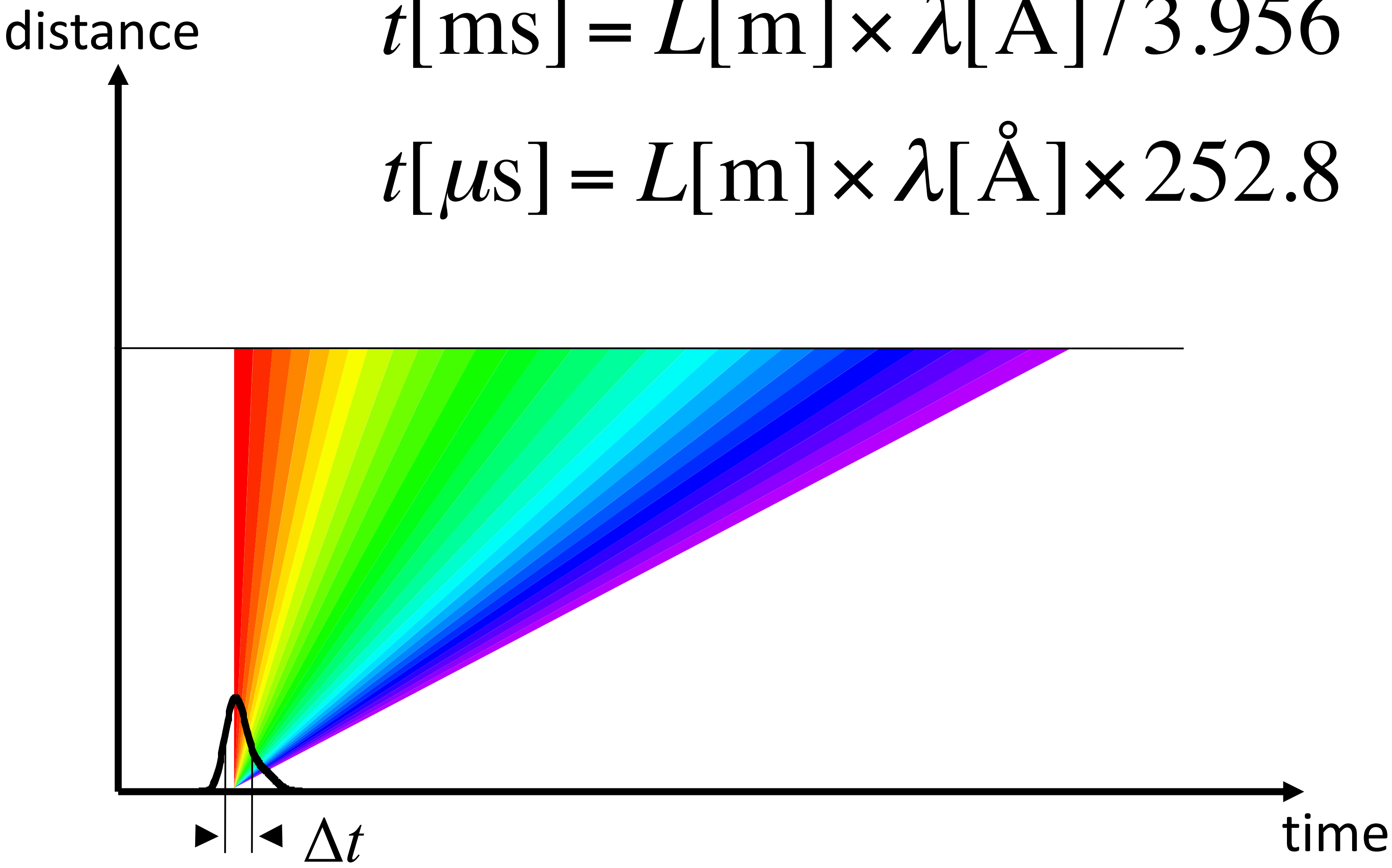
Varying **angle** to access different Q values

Varying **angle and wavelength** to access different Q values

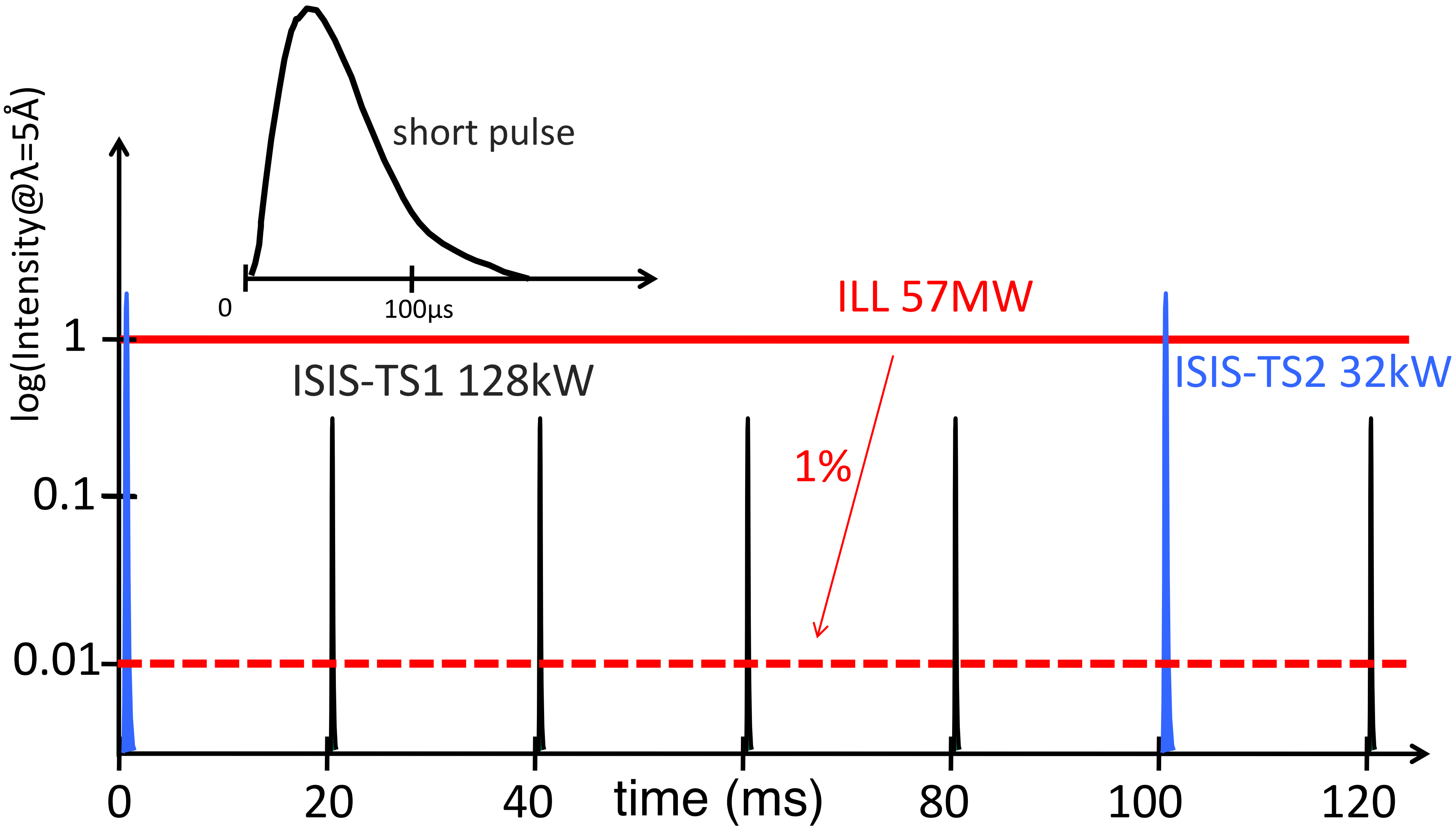
The Time-of-Flight (TOF) Method

$$t[\text{ms}] = L[\text{m}] \times \lambda[\text{Å}] / 3.956$$

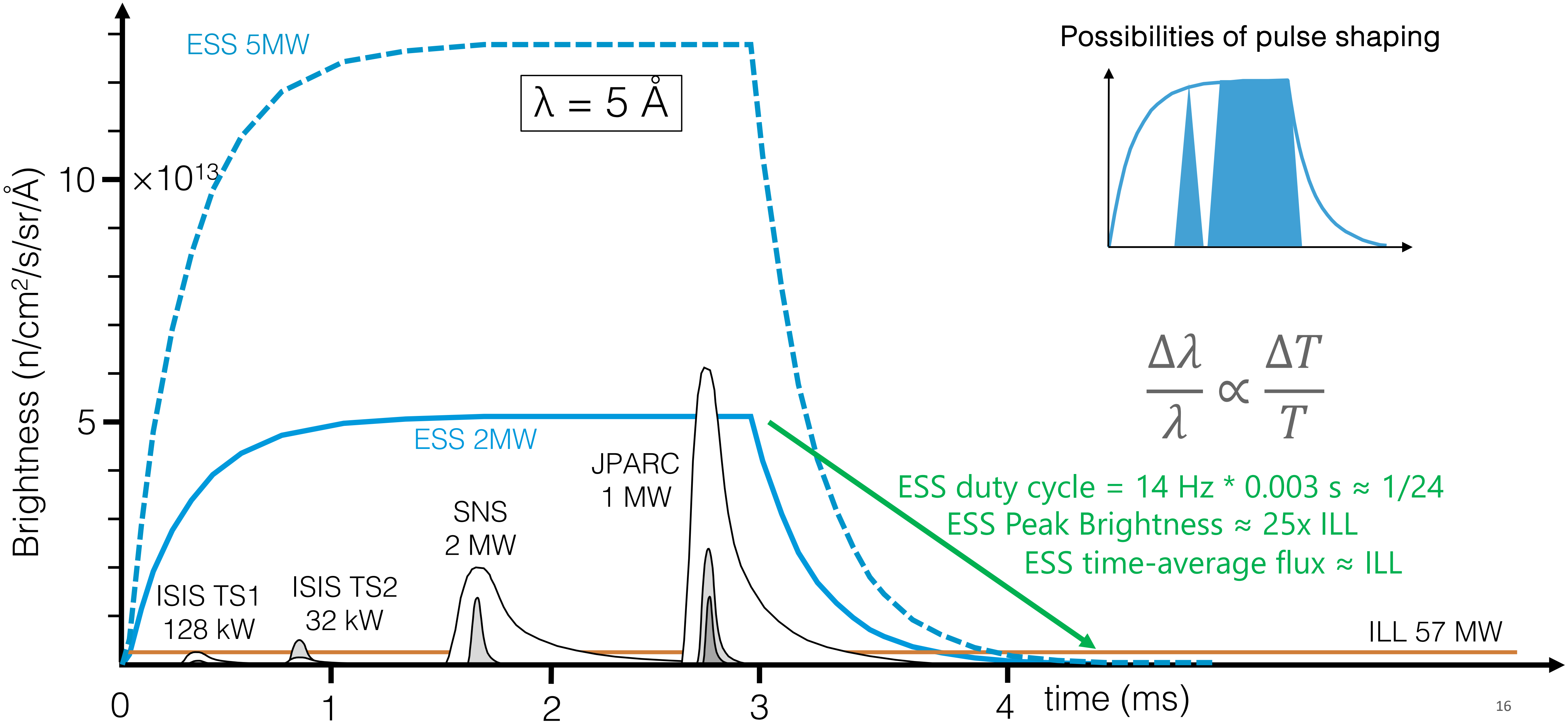
$$t[\mu\text{s}] = L[\text{m}] \times \lambda[\text{Å}] \times 252.8$$



Pulsed source time structures (λ=5Å)



Long-pulse Performance and Flexibility



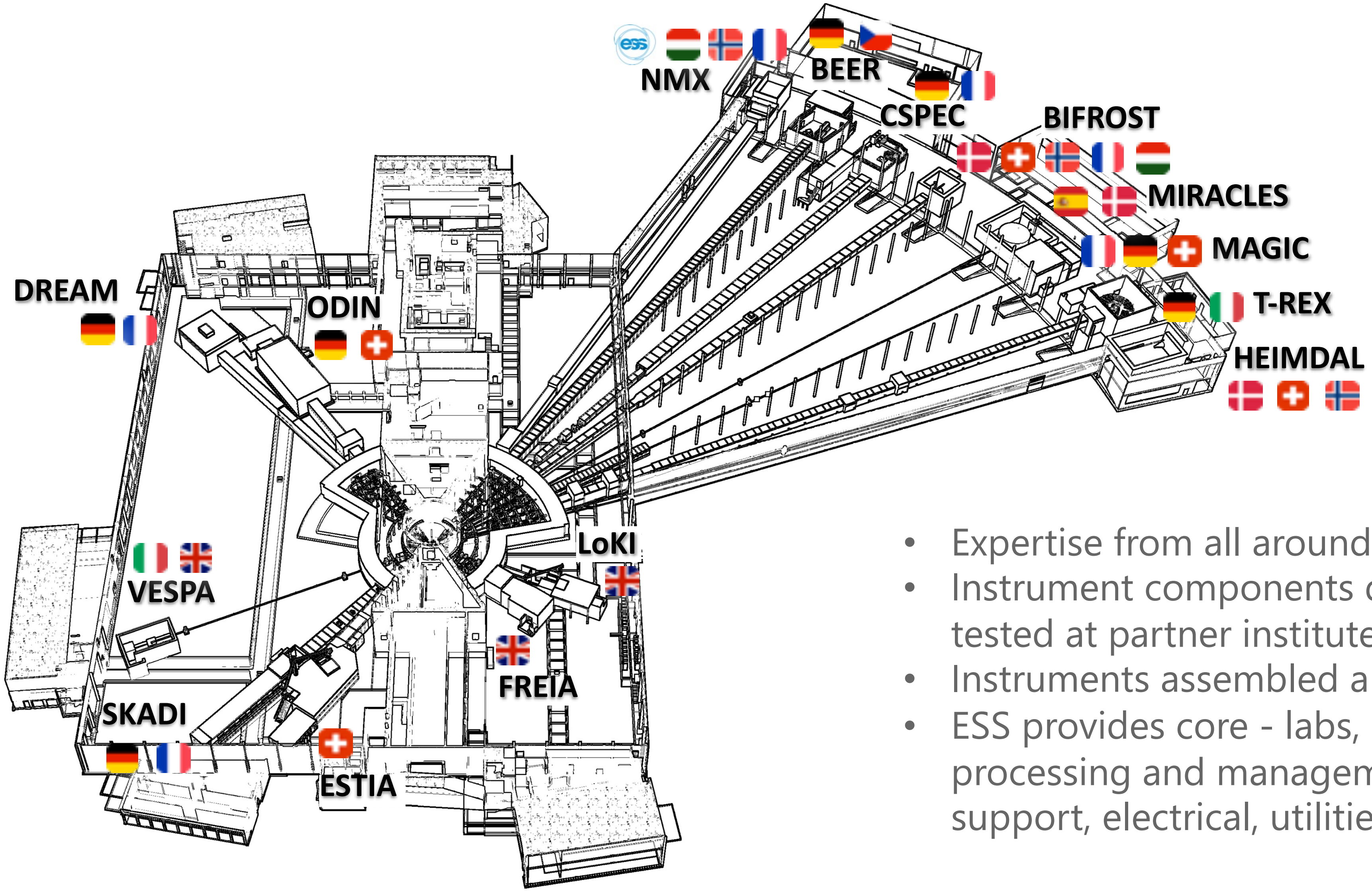
Possibilities of pulse shaping

$$\frac{\Delta\lambda}{\lambda} \propto \frac{\Delta T}{T}$$

ESS duty cycle = 14 Hz * 0.003 s ≈ 1/24
ESS Peak Brightness ≈ 25x ILL
ESS time-average flux ≈ ILL

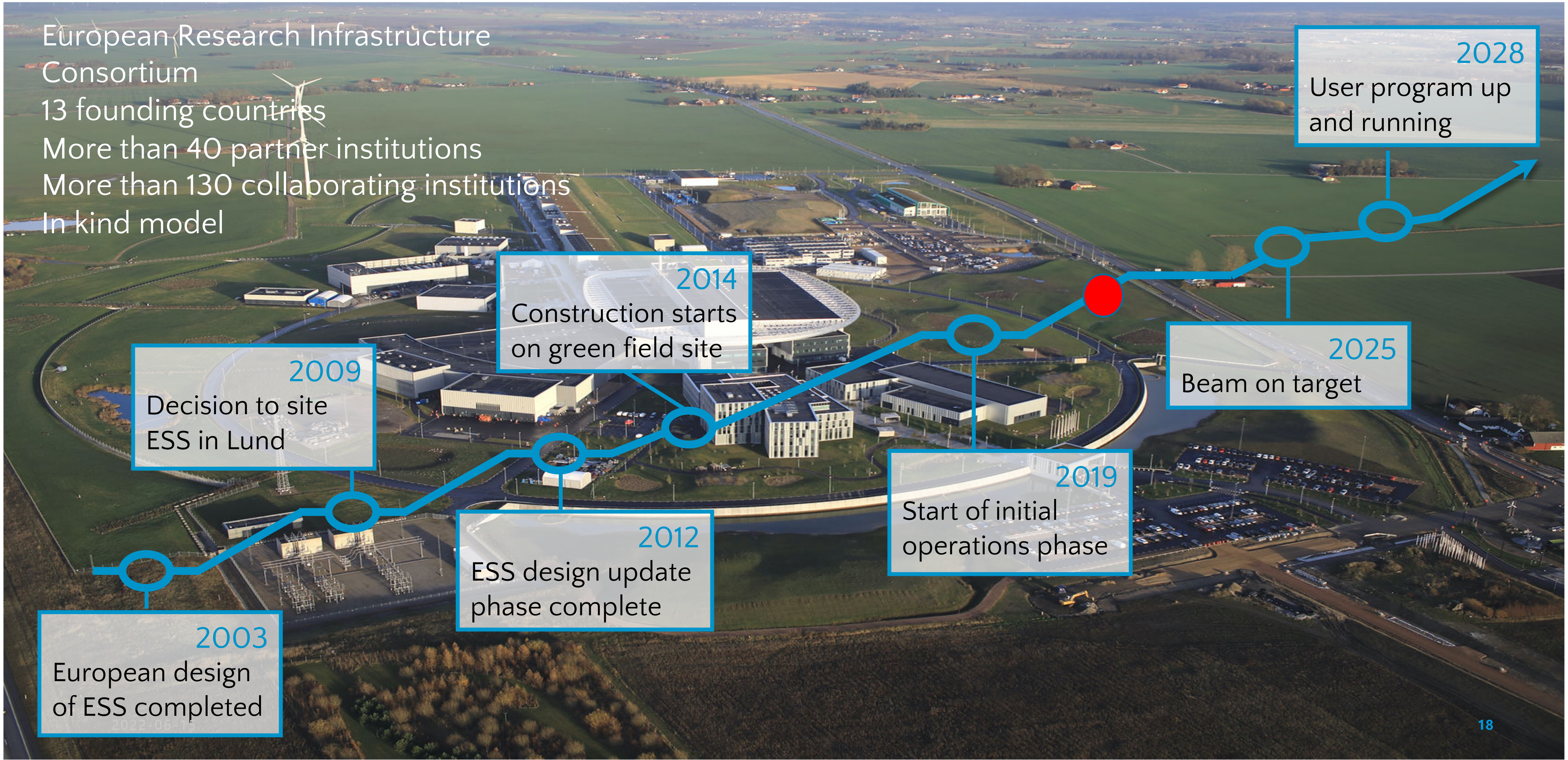
Neutron Science Instruments at ESS

1 Imaging, 2 SANS, 2 Reflectometers, 5 Spectrometers, 5 Diffractometers, 1 Test Beamline



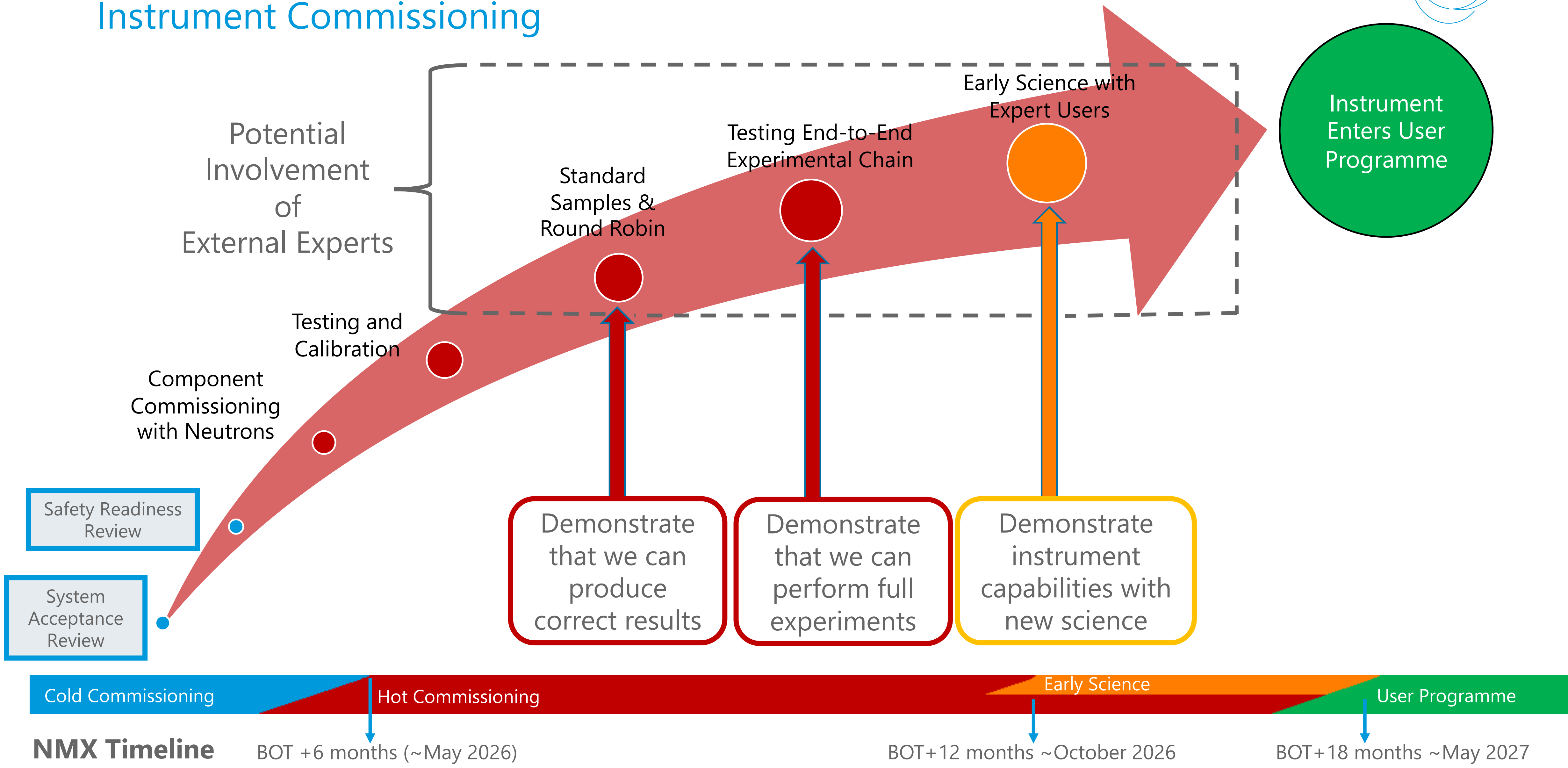
- Expertise from all around Europe
- Instrument components designed, built, and tested at partner institutes
- Instruments assembled and integrated at ESS
- ESS provides core - labs, data acquisition, processing and management, engineering support, electrical, utilities, safety systems,

The ESS journey



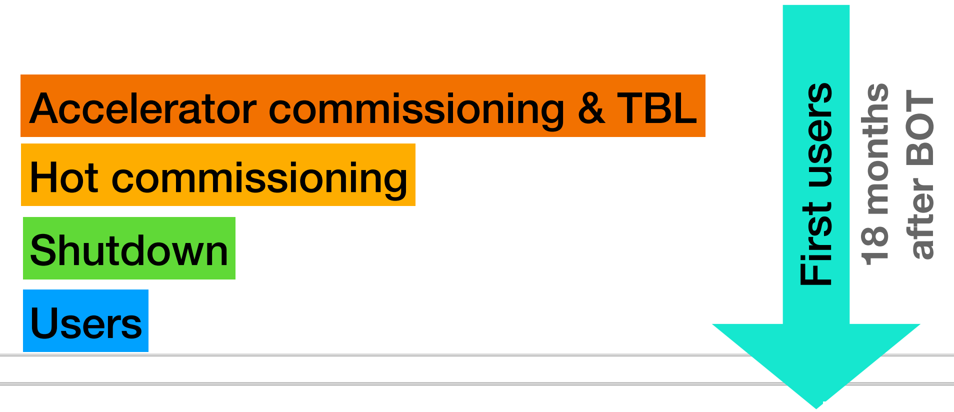
Towards the User Programme

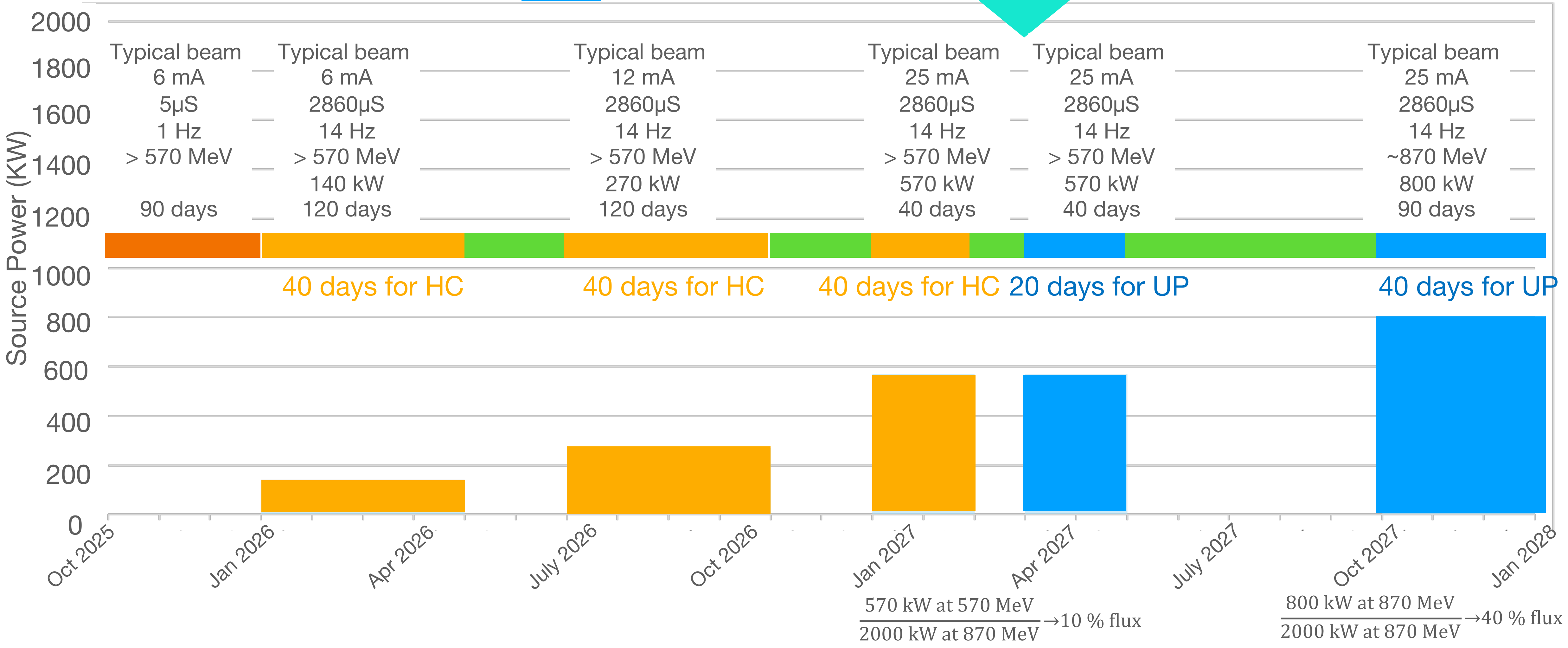
Instrument Commissioning



ESS Ramp up

Assuming BOT July 2025





Summary

NMX is expected to be ready for early science commissioning experiments in late 2026 and user programme access by mid 2027

Now is time to think about what experiments might be done and begin collaborations and sample preparation

I look forward to hearing the ideas today!