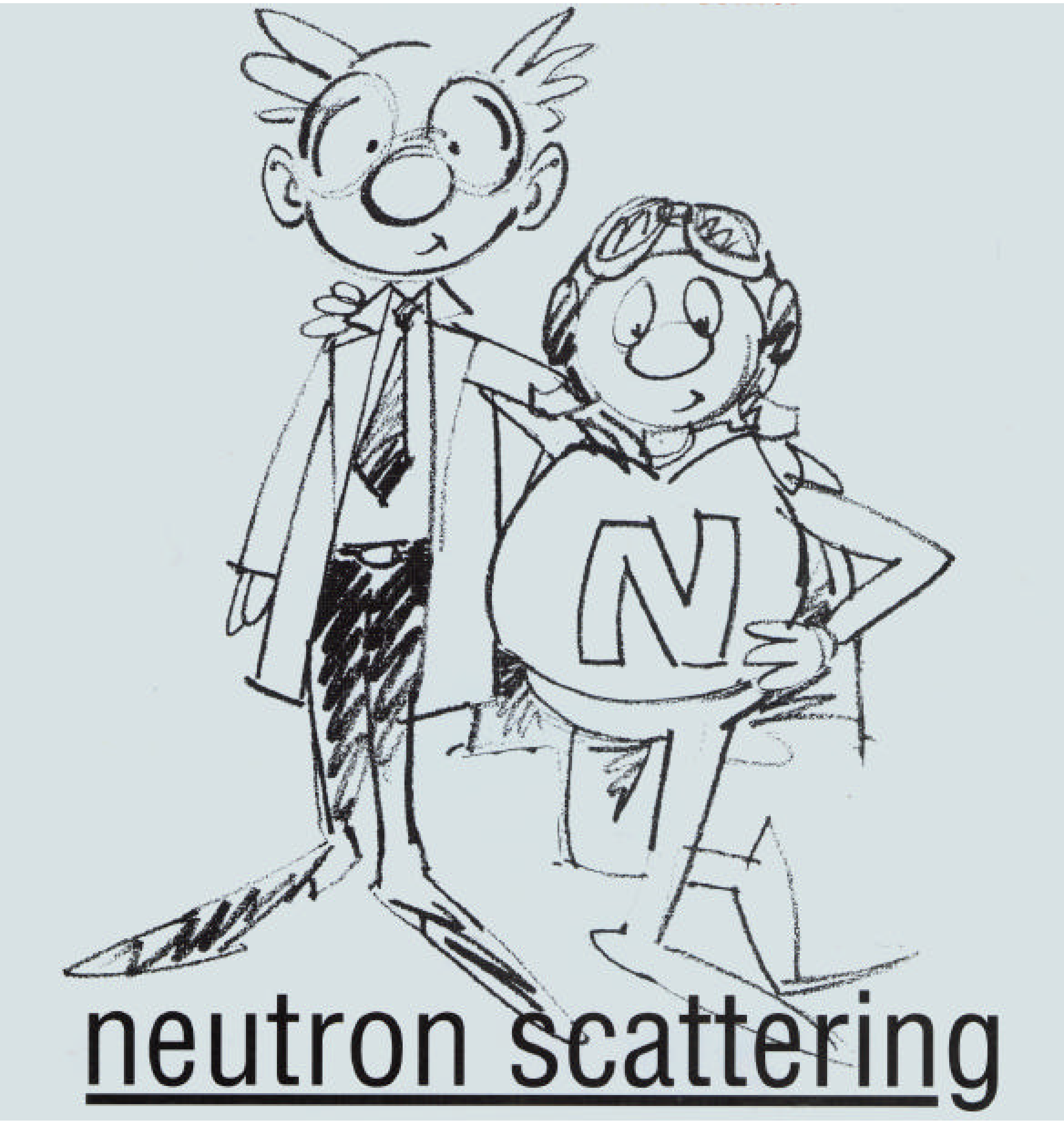


by

Roger Pynn

Los Alamos
National Laboratory

LECTURE 2: Neutron Scattering Instrumentation & Facilities

Overview

1. Essential messages from Lecture #1
2. Neutron Scattering Instrumentation and Facilities – how is neutron scattering measured?
    1. Sources of neutrons for scattering – reactors & spallation sources
        1. Neutron spectra
        2. Monochromatic-beam and time-of-flight methods
    2. Instrument components
    3. A “zoo” of specialized neutron spectrometers

Recapitulation of Key Messages From Lecture #1

- Neutron scattering experiments measure the number of neutrons scattered by a sample as a function of the wavevector change (Q) and the energy change (E) of the neutron

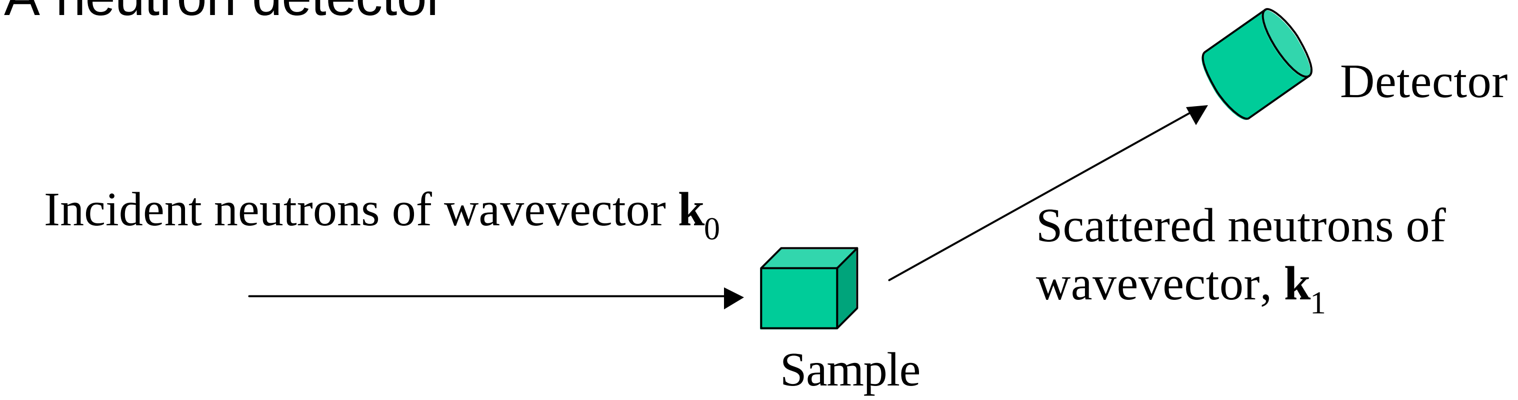
- Expressions for the scattered neutron intensity involve the positions and motions of atomic nuclei or unpaired electron spins in the scattering sample

- The scattered neutron intensity as a function of Q and E is proportional to the space and time Fourier Transform of the probability of finding two atoms separated by a particular distance at a particular time

- Sometimes the change in the spin state of the neutron during scattering is also measured to give information about the locations and orientations of unpaired electron spins in the sample

What Do We Need to Do a Basic Neutron Scattering Experiment?

- A source of neutrons
- A method to prescribe the wavevector of the neutrons incident on the sample
- (An interesting sample)
- A method to determine the wavevector of the scattered neutrons
  - Not needed for elastic scattering
- A neutron detector

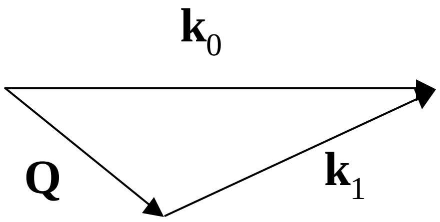


Detector

Incident neutrons of wavevector $\mathbf{k}_0$

Scattered neutrons of wavevector, $\mathbf{k}_1$

Sample



$\mathbf{k}_0$

$\mathbf{Q}$

$\mathbf{k}_1$

Remember: wavevector, k, & wavelength, λ, are related by: $k = m_n v/(h/2\pi) = 2\pi/\lambda$

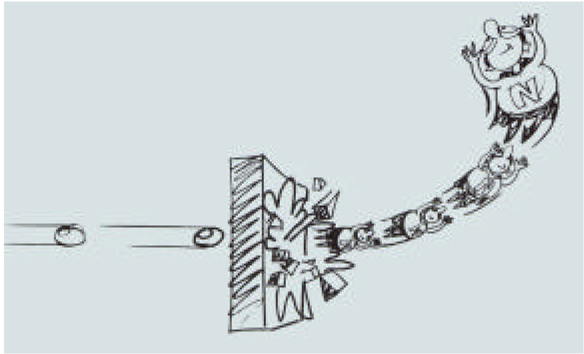
Neutron Scattering Requires Intense Sources of Neutrons

- Neutrons for scattering experiments can be produced either by nuclear fission in a reactor or by spallation when high-energy protons strike a heavy metal target (W, Ta, or U).
  - In general, reactors produce continuous neutron beams and spallation sources produce beams that are pulsed between 20 Hz and 60 Hz
  - The energy spectra of neutrons produced by reactors and spallation sources are different, with spallation sources producing more high-energy neutrons
  - Neutron spectra for scattering experiments are tailored by moderators – solids or liquids maintained at a particular temperature – although neutrons are not in thermal equilibrium with moderators at a short-pulse spallation sources

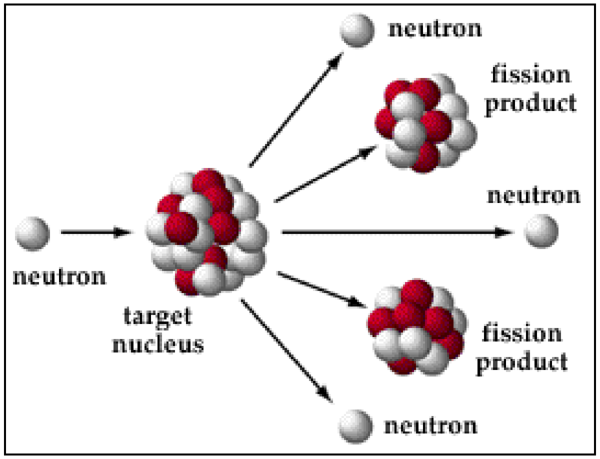
- Both reactors and spallation sources are expensive to build and require sophisticated operation.
  - SNS at ORNL will cost about $1.5B to construct & ~$140M per year to operate

- Either type of source can provide neutrons for 30-50 neutron spectrometers
  - Small science at large facilities

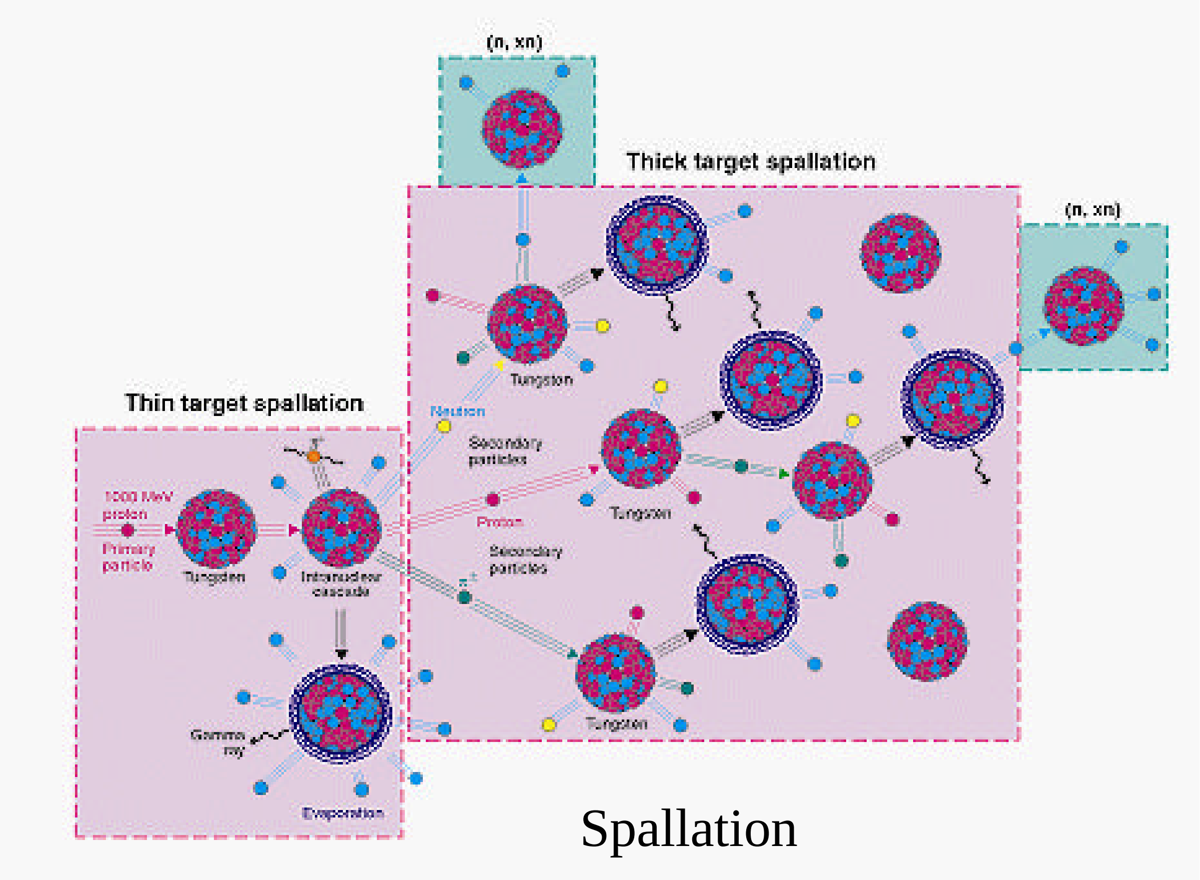
About 1.5 Useful Neutrons Are Produced by Each Fission Event in a Nuclear Reactor Whereas About 25 Neutrons Are Produced by spallation for Each 1-GeV Proton Incident on a Tungsten Target



Artist's view of spallation



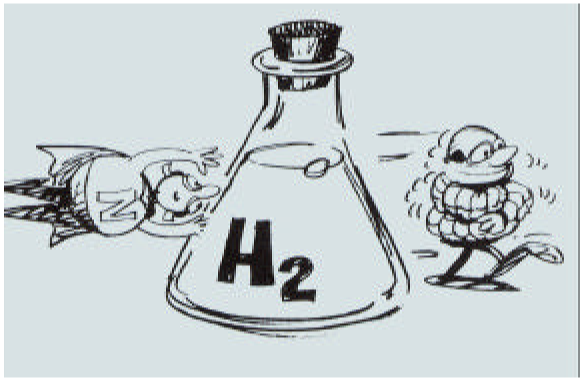
Nuclear Fission

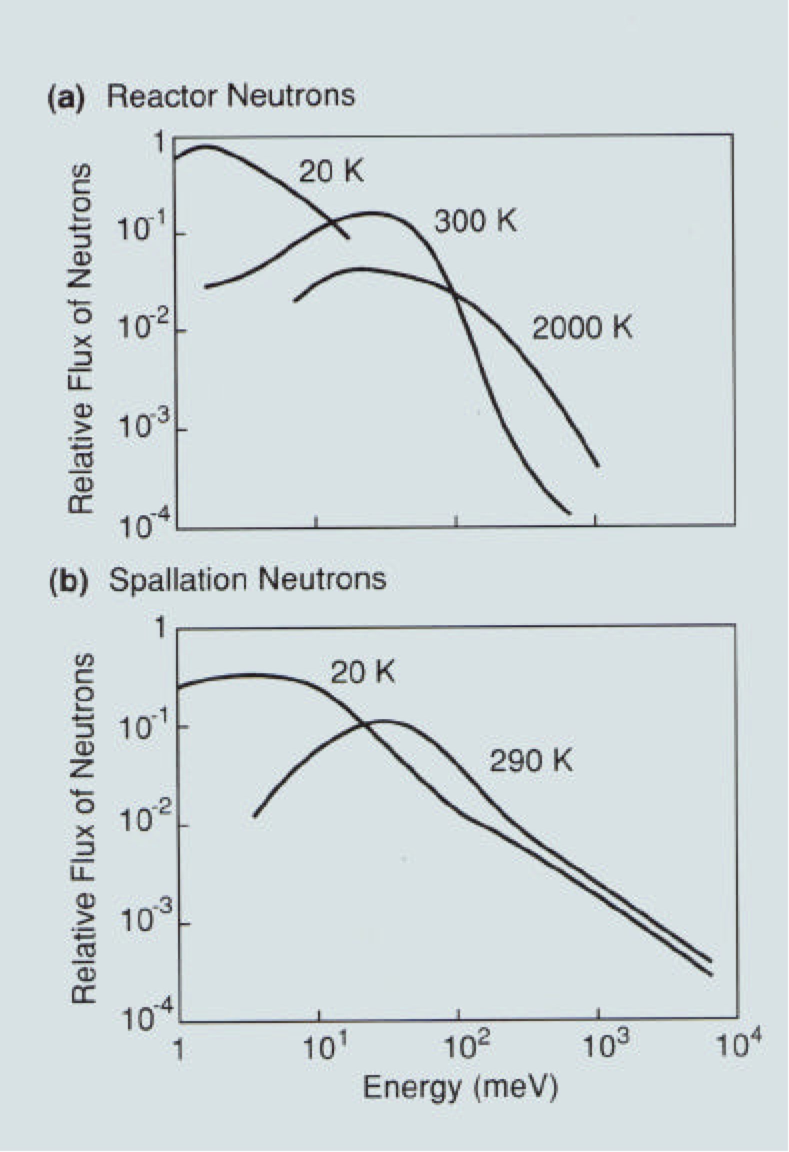


Spallation

Neutrons From Reactors and Spallation Sources Must Be Moderated Before Being Used for Scattering Experiments

- Reactor spectra are Maxwellian
- Intensity and peak-width ~ $1/(E)^{1/2}$ at high neutron energies at spallation sources
- Cold sources are usually liquid hydrogen (though deuterium is also used at reactors & methane is sometimes used at spallation sources)
- Hot source at ILL (only one in the world) is graphite, radiation heated.



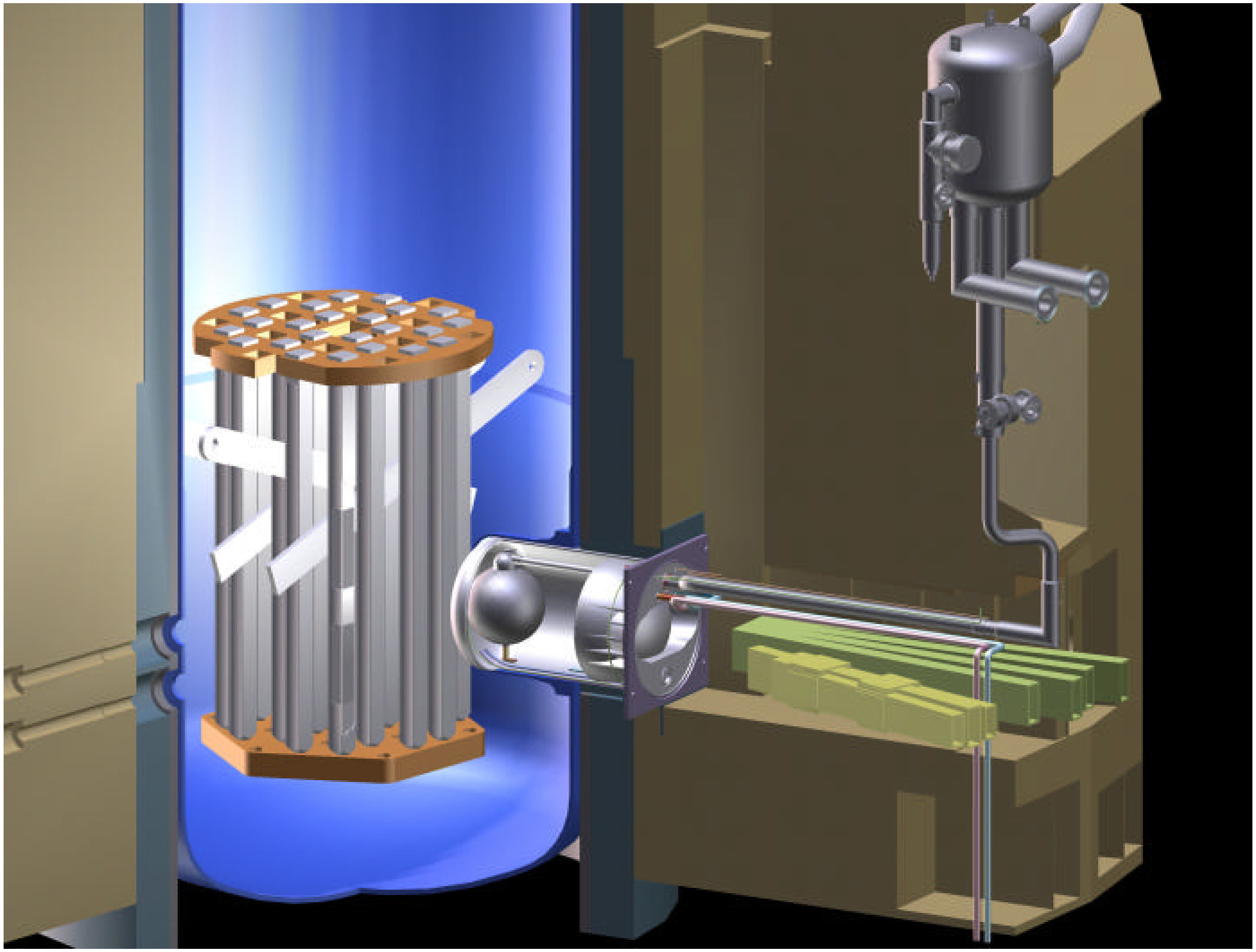


The ESRF* & ILL* With Grenoble & the Beldonne Mountains

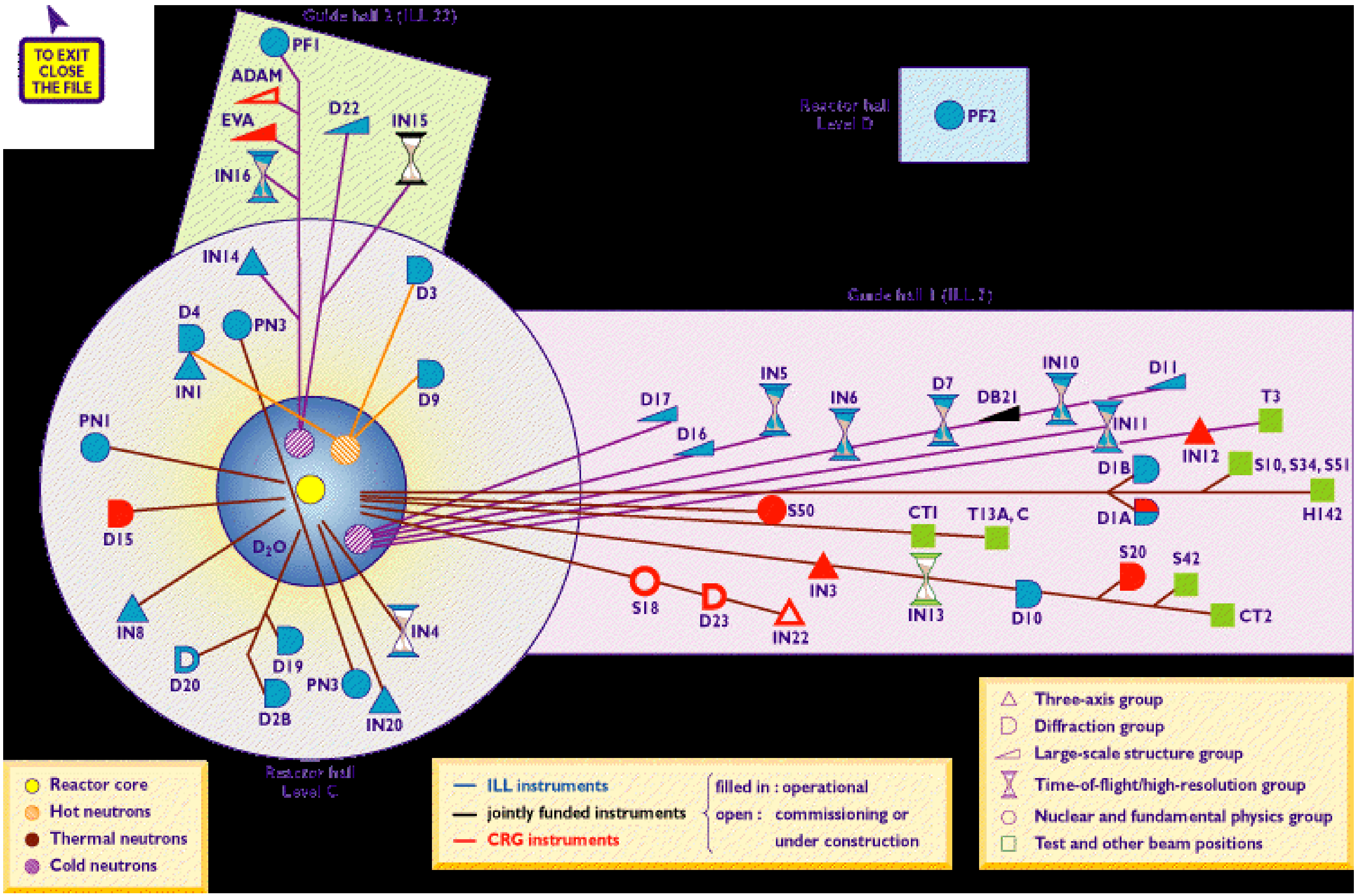
Photo ESRF/Studio de la Revirée

*ESRF = European Synchrotron Radiation Facility; ILL = Institut Laue-Langevin

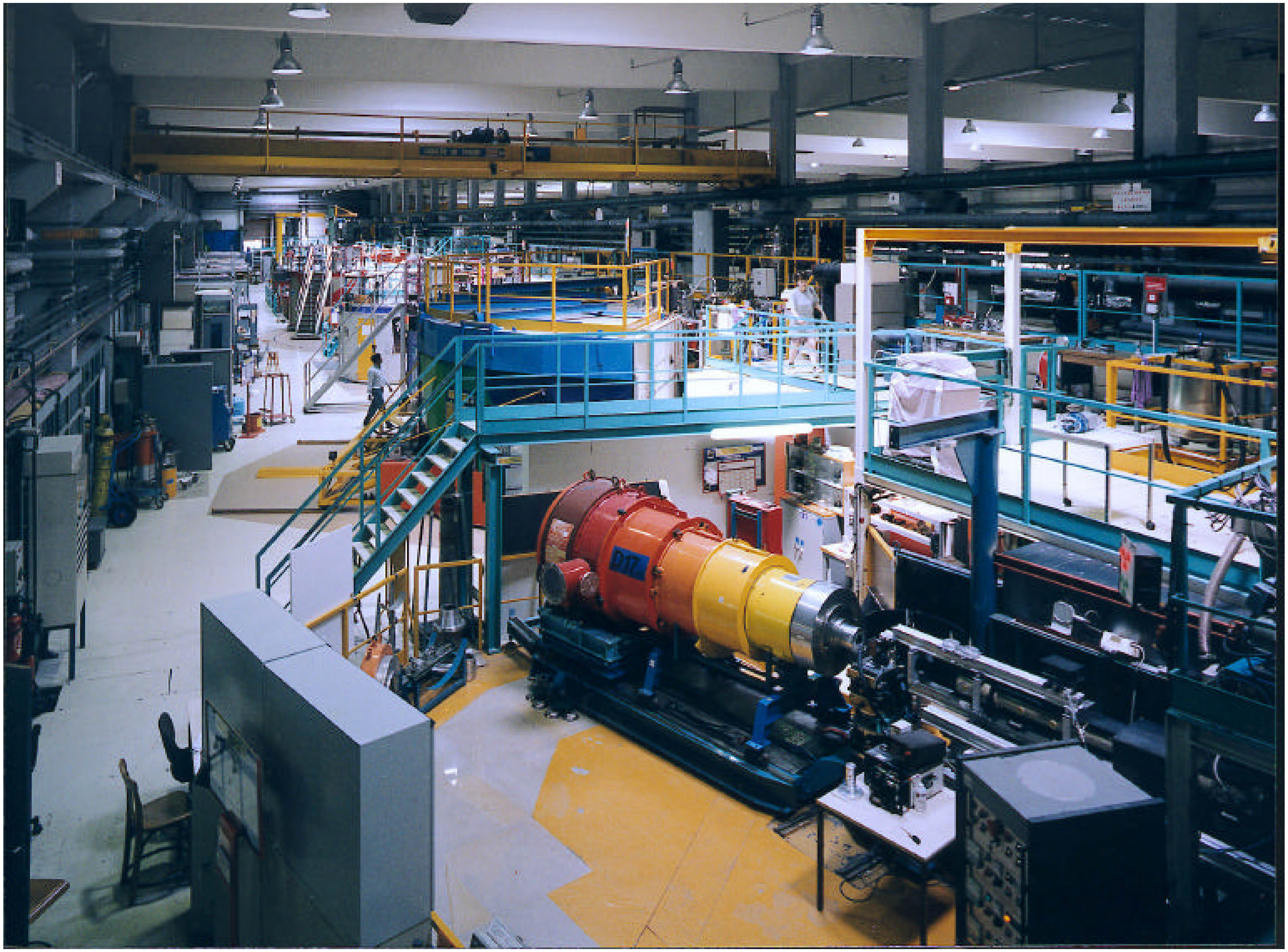
The National Institute of Standards and Technology (NIST) Reactor Is a 20 MW Research Reactor With a Peak Thermal Flux of 4×10^{14} N/sec. It Is Equipped With a Unique Liquid-hydrogen Moderator That Provides Neutrons for Seven Neutron Guides



Neutron Sources Provide Neutrons for Many Spectrometers: Schematic Plan of the ILL Facility



A ~ 30 X 20 m^2 Hall at the ILL Houses About 30 Spectrometers. Neutrons Are Provided Through Guide Tubes



Los Alamos Neutron Science Center

Manuel Lujan Jr.
Neutron Scattering
Center

Proton
Radiography

Proton Storage
Ring

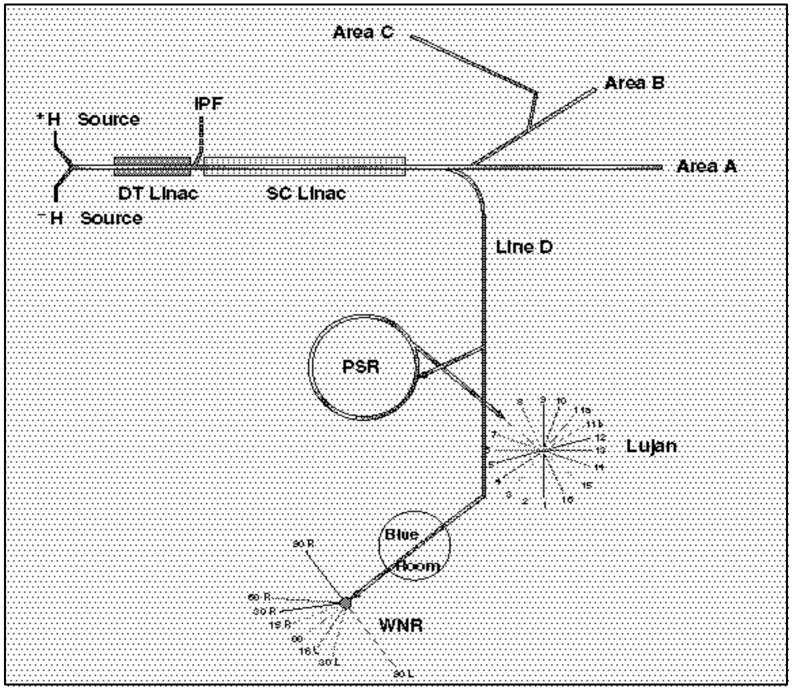
Weapons
Neutron Research

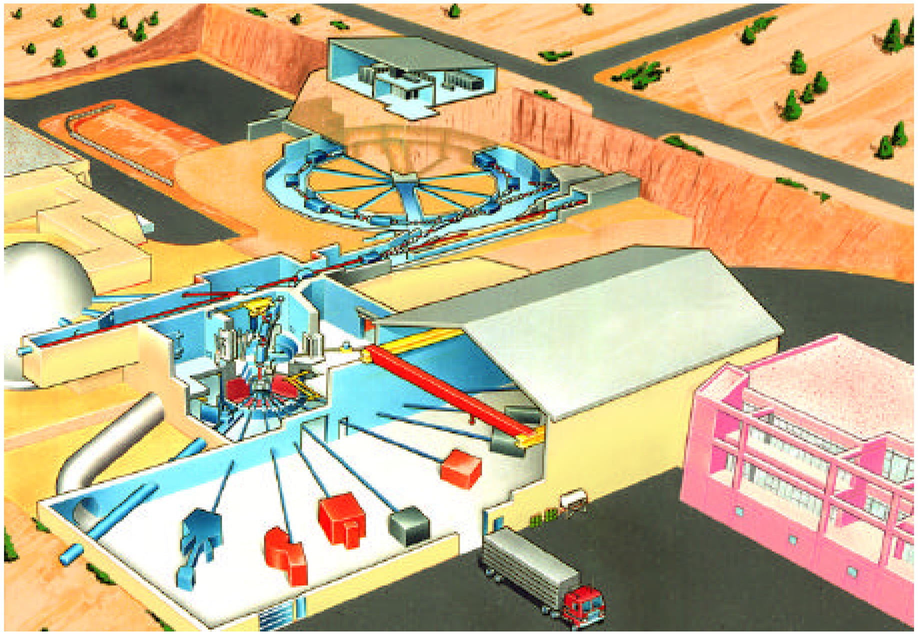
800-MeV Linear
Accelerator

LANSCE
Visitor's Center

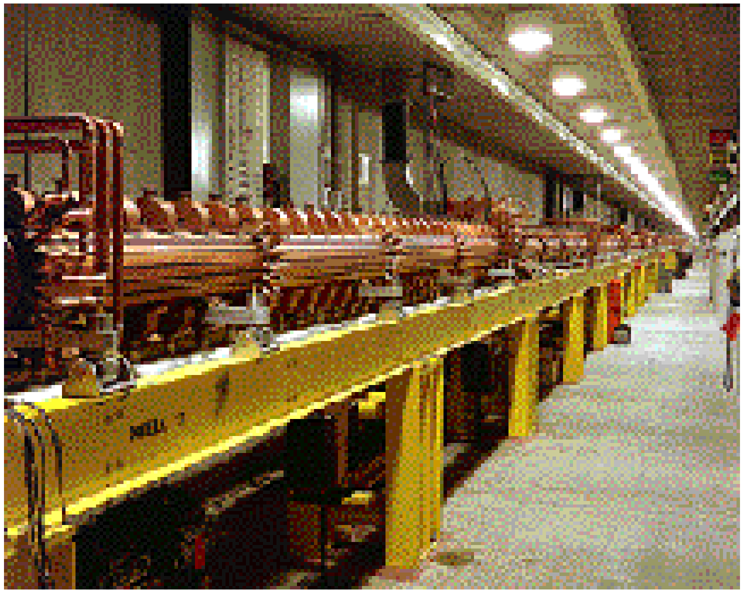
Neutron Production at LANSCE

- Linac produces 20 H^- (a proton + 2 electrons) pulses per second
  - 800 MeV, ~800 µsec long pulses, average current ~100 µA
- Each pulse consists of repetitions of 270 nsec on, 90 nsec off
- Pulses are injected into a Proton Storage Ring with a period of 360 nsec
  - Thin carbon foil strips electrons to convert H^- to H^+ (I.e. a proton)
  - ~3 x 10^{13} protons/pulse ejected onto neutron production target

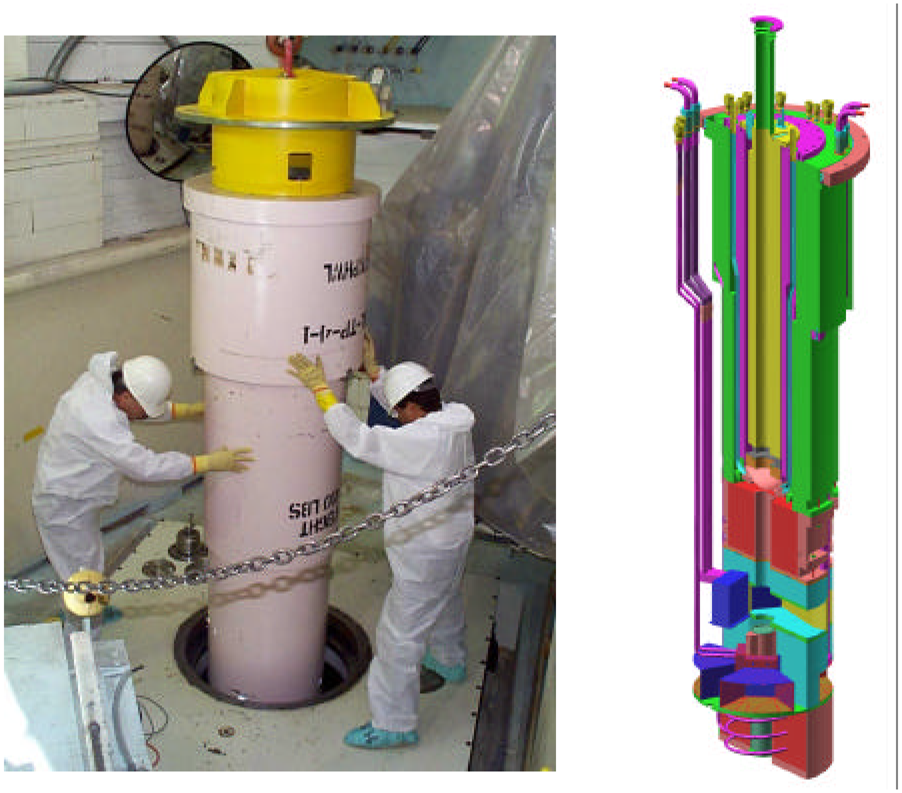




Components of a Spallation Source



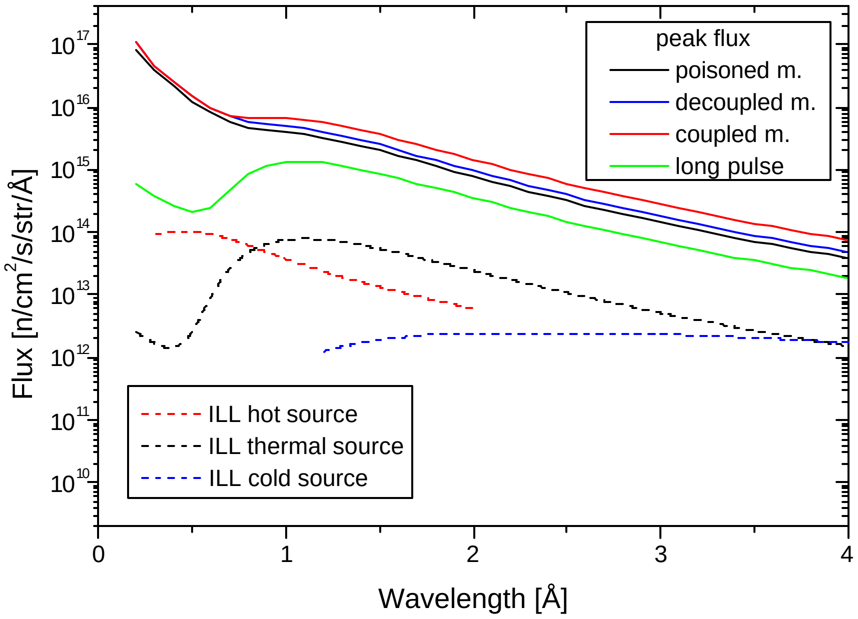
A half-mile long proton linac…

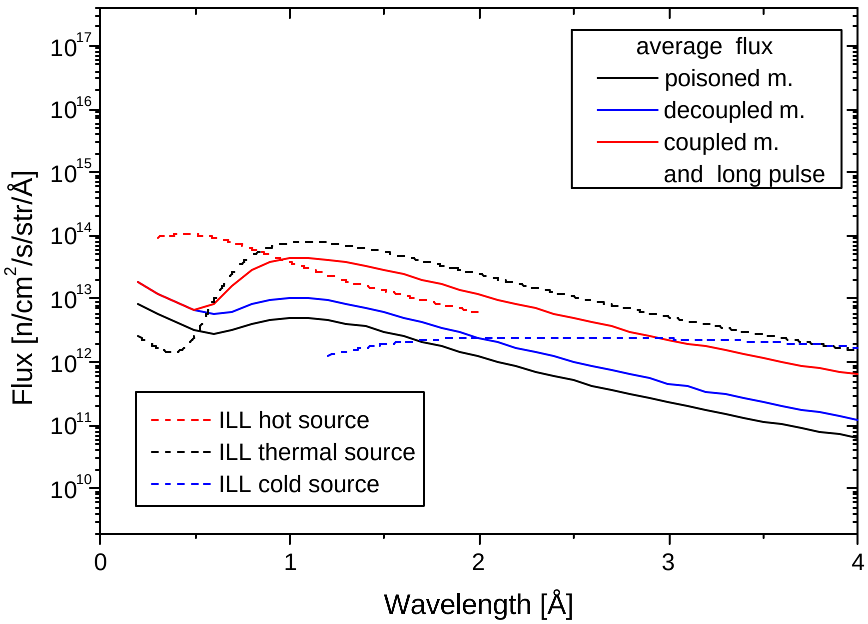


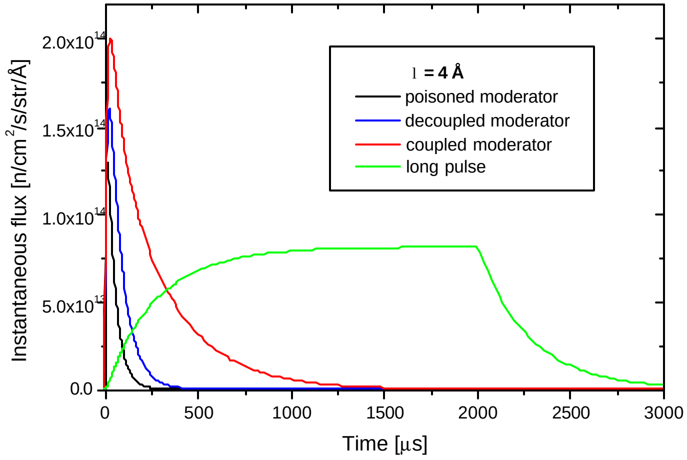
…and a neutron production target

….a proton accumulation ring….

A Comparison of Neutron Flux Calculations for the ESS SPSS (50 Hz, 5 MW) & LPSS (16 Hz, 5W) With Measured Neutron Fluxes at the ILL

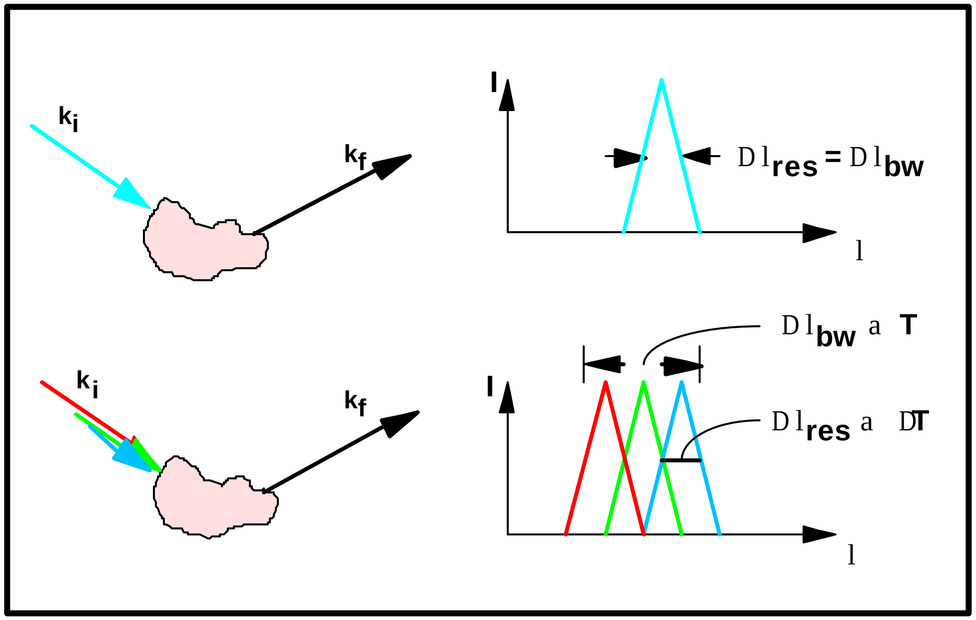


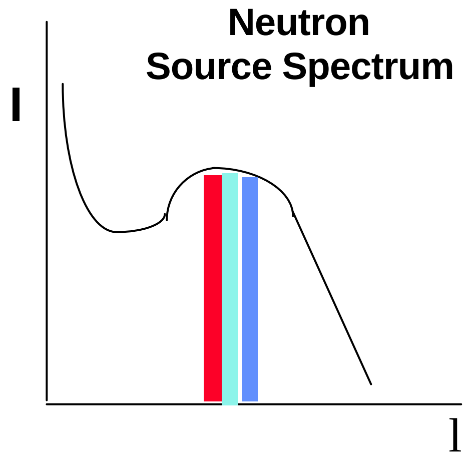




Pulsed sources only make sense if one can make effective use of the flux in each pulse, rather than the average neutron flux

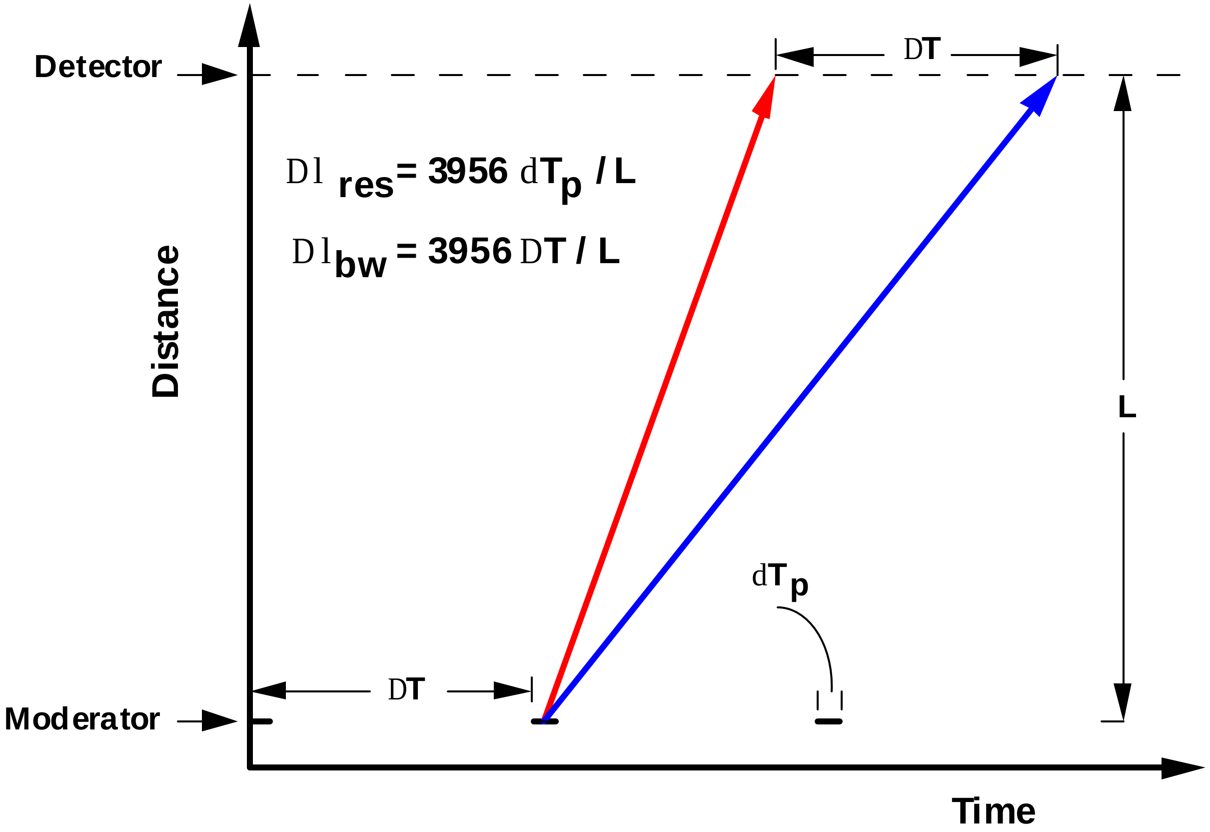
Simultaneously Using Neutrons With Many Different Wavelengths Enhances the Efficiency of Neutron Scattering Experiments





Potential Performance Gain relative to use of a Single Wavelength is the Number of Different Wavelength Slices used

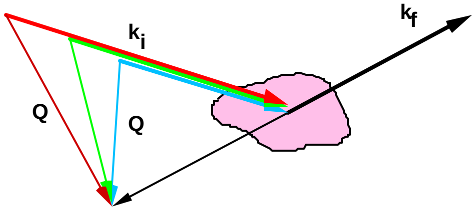
The Time-of-flight Method Uses Multiple Wavelength Slices at a Reactor or a Pulsed Spallation Source



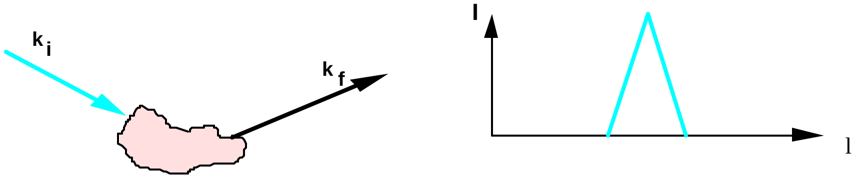
When the neutron wavelength is determined by time-of-flight, $\Delta T/\delta T_p$ different wavelength slices can be used simultaneously.

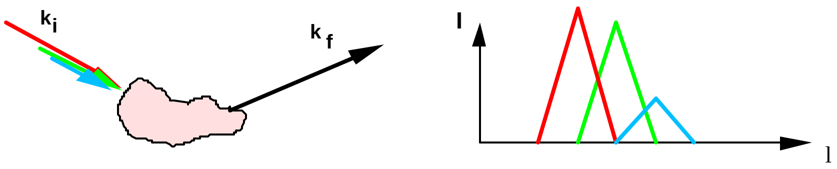
The Actual ToF Gain From Source Pulsing
Often Does Not Scale Linearly With Peak Neutron Flux

low rep. rate => large dynamic range
short pulse => good resolution —
neither may be necessary or useful

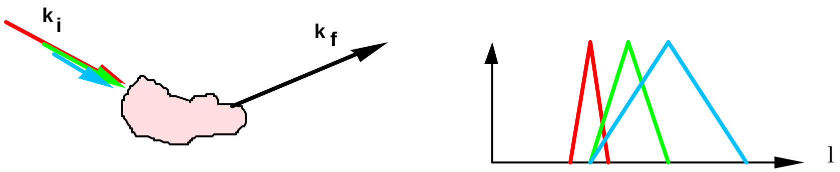


large dynamic range may result in intensity changes across the spectrum





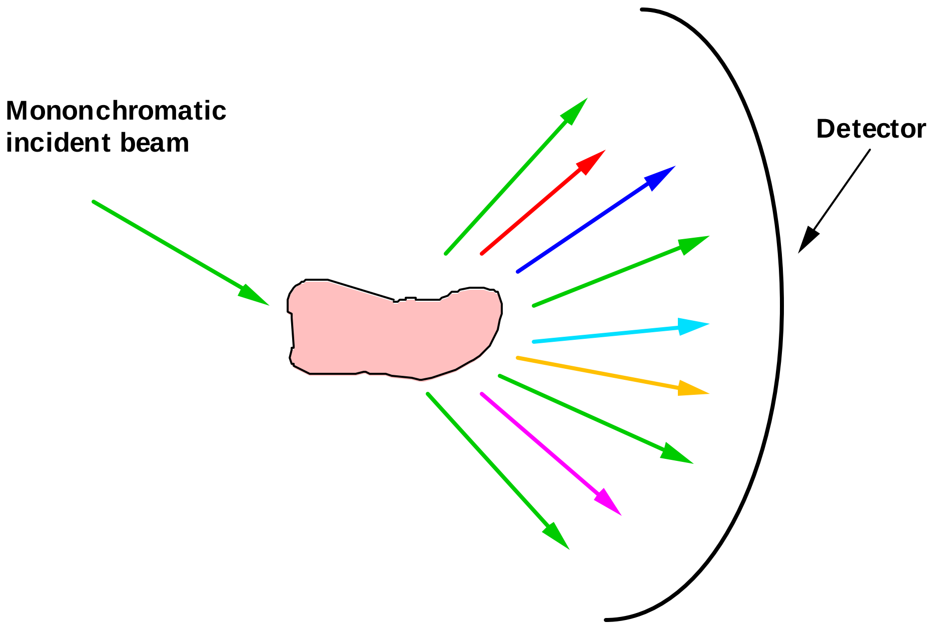
at a traditional short-pulse source the wavelength resolution changes with wavelength



A Comparison of Reactors & Spallation Sources

Short Pulse Spallation Source	Reactor
Energy deposited per useful neutron is ~20 MeV	Energy deposited per useful neutron is ~ 180 MeV
Neutron spectrum is “slowing down” spectrum – preserves short pulses	Neutron spectrum is Maxwellian
Constant, small $\delta\lambda/\lambda$ at large neutron energy => excellent resolution especially at large Q and E	Resolution can be more easily tailored to experimental requirements, except for hot neutrons where monochromator crystals and choppers are less effective
Copious “hot” neutrons=> very good for measurements at large Q and E	Large flux of cold neutrons => very good for measuring large objects and slow dynamics
Low background between pulses => good signal to noise	Pulse rate for TOF can be optimized independently for different spectrometers
Single pulse experiments possible	Neutron polarization easier

Why Isn’t There a Universal Neutron Scattering Spectrometer?



Elastic Scattering — detect all scattered neutrons

Inelastic Scattering — detect neutrons as a function of scattered energy (color)

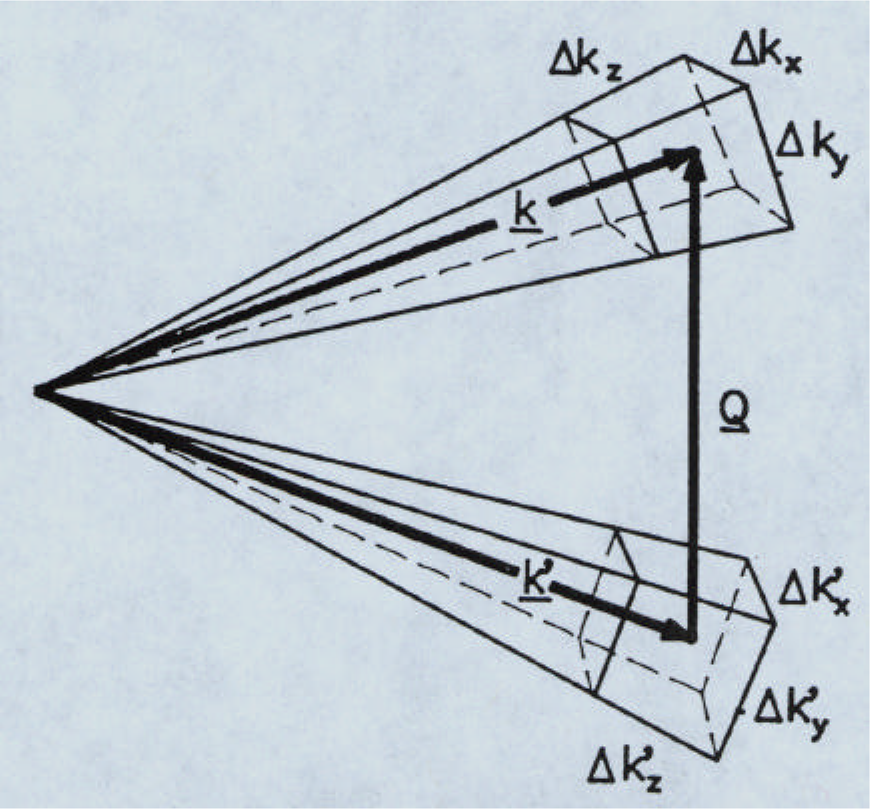
- Conservation of momentum => $\underline{Q} = \underline{k}_f - \underline{k}_i$
- Conservation of energy => $E = (h^2 m/ 8 p^2) (k_f^2 - k_i^2)$
- Scattering properties of sample depend only on Q and E, not on neutron l

Many types of neutron scattering spectrometer are required because the accessible Q and E depend on neutron energy and because resolution and detector coverage have to be tailored to the science for such a signal-limited technique.

Brightness & Fluxes for Neutron & X-ray Sources

	Brightness (s^{-1} m^{-2} $ster^{-1}$)	*dE/E (%)*	*Divergence ($mrad^2$)*	*Flux (s^{-1} m^{-2})*
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5×10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5×10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01 x 0.1	10^{24}

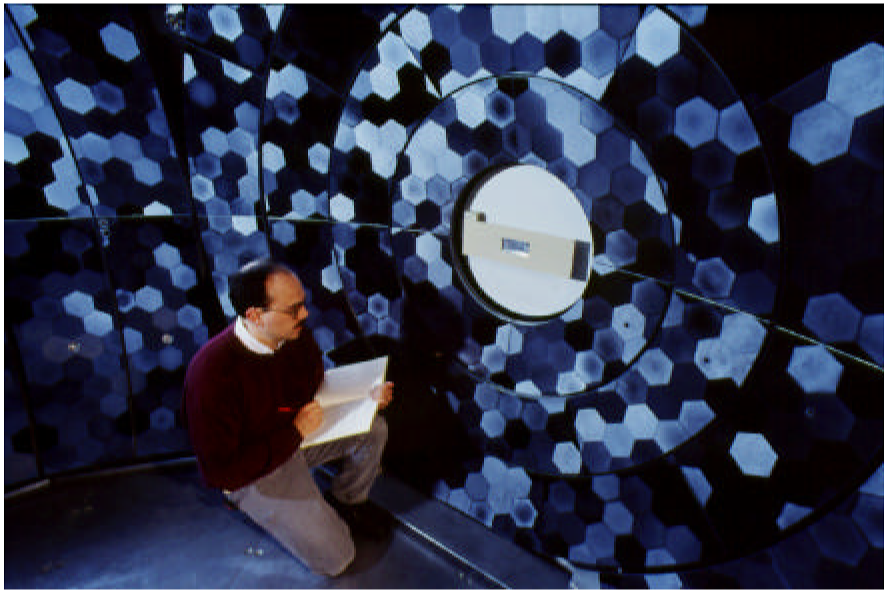
Instrumental Resolution



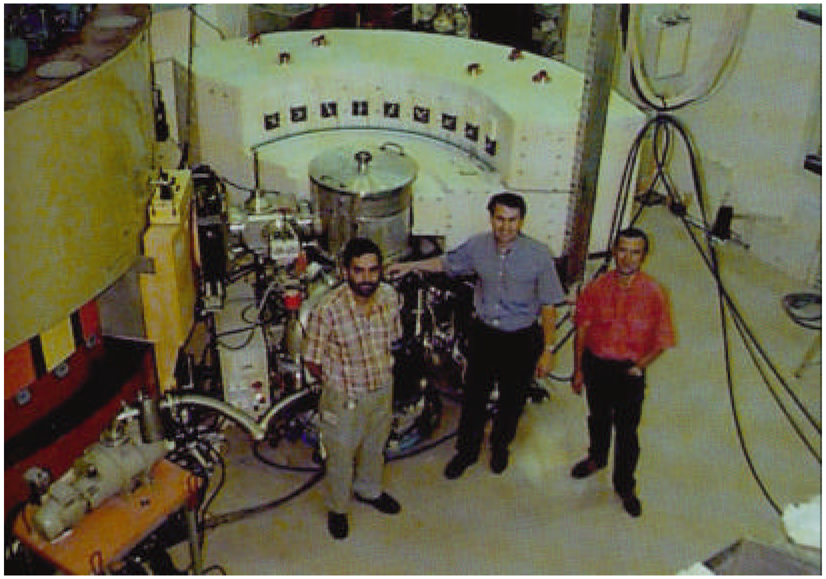
- Uncertainties in the neutron wavelength & direction of travel imply that Q and E can only be defined with a certain precision
- When the box-like resolution volumes in the figure are convolved, the overall resolution is Gaussian (central limit theorem) and has an elliptical shape in (Q,E) space
- The total signal in a scattering experiment is proportional to the phase space volume within the elliptical resolution volume – the better the resolution, the lower the count rate

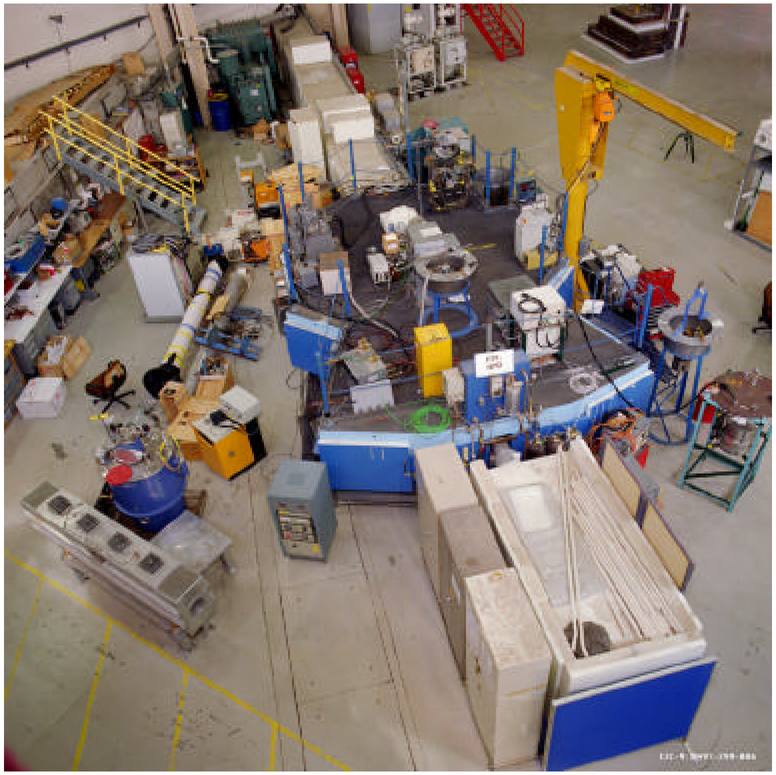
Examples of Specialization of Spectrometers: Optimizing the Signal for the Science

- Small angle scattering [$Q = 4\pi \sin\theta/\lambda$; $(\delta Q/Q)^2 = (\delta\lambda/\lambda)^2 + (\cot\theta\ \delta\theta)^2$]
  - Small diffraction angles to observe large objects => long (20 m) instrument
  - poor monochromatization ($\delta\lambda/\lambda \sim 10\%$) sufficient to match obtainable angular resolution (1 cm^2 pixels on 1 m^2 detector at 10 m => $\delta\theta \sim 10^{-3}$ at $\theta \sim 10^{-2}$))
- Back scattering [$\theta = \pi/2$; $\lambda = 2\, d \sin\,\theta$; $\delta\lambda/\lambda = \cot\,\theta + \ldots$]
  - very good energy resolution (~neV) => perfect crystal analyzer at $\theta \sim \pi/2$
  - poor Q resolution => analyzer crystal is very large (several m^2)



Typical Neutron Scattering Instruments





Note: relatively massive shielding; long flight paths for time-of-flight spectrometers; many or multi-detectors

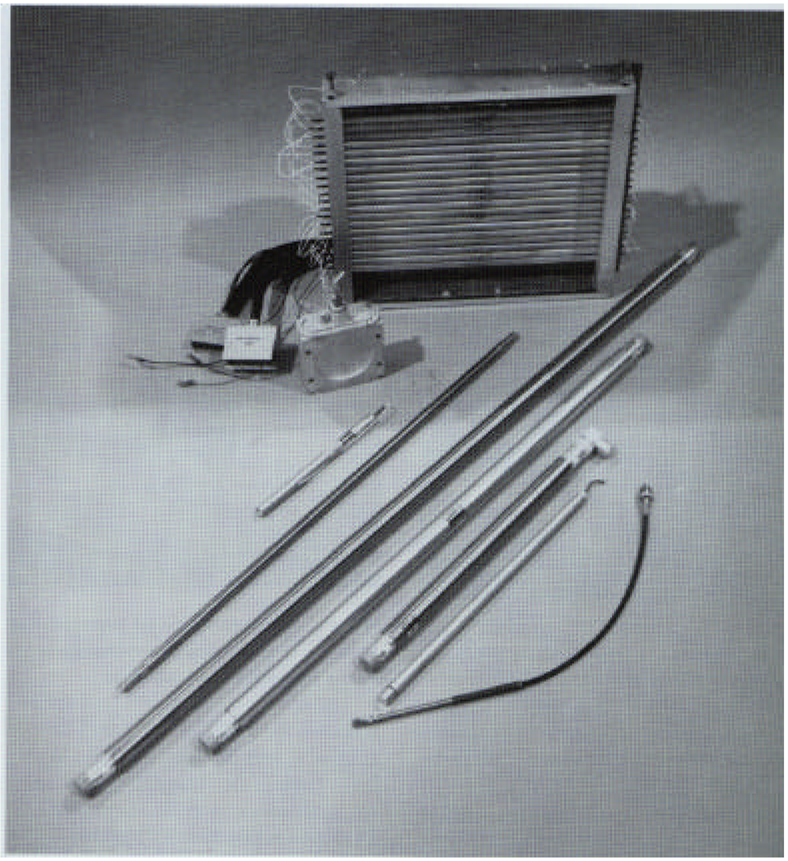
but… small science at a large facility

Components of Neutron Scattering Instruments

- Monochromators
  - Monochromate or analyze the energy of a neutron beam using Bragg's law
- Collimators
  - Define the direction of travel of the neutron
- Guides
  - Allow neutrons to travel large distances without suffering intensity loss
- Detectors
  - Neutron is absorbed by ^{3}He and gas ionization caused by recoiling particles is detected
- Choppers
  - Define a short pulse or pick out a small band of neutron energies
- Spin turn coils
  - Manipulate the neutron spin using Lamor precession
- Shielding
  - Minimize background and radiation exposure to users

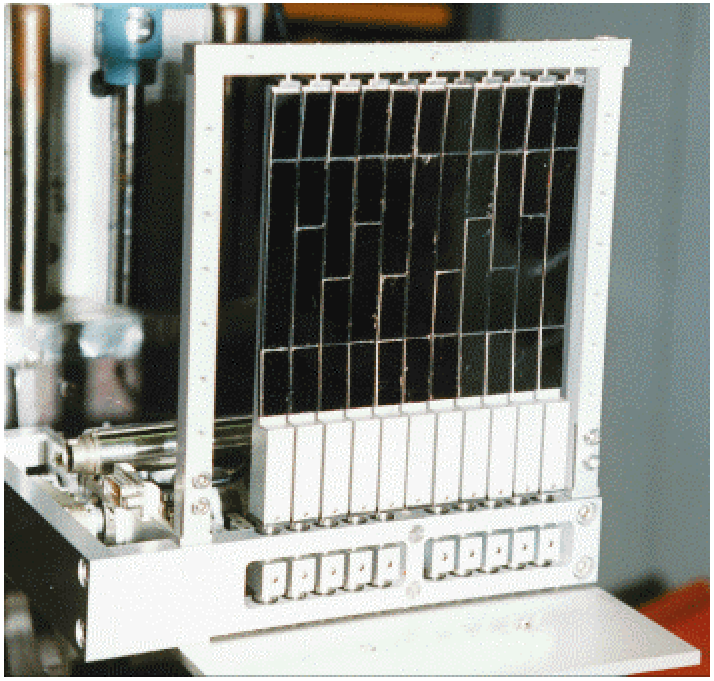
Most Neutron Detectors Use ^{3}He

- ^{3}He + n -> ^{3}H + p + 0.764 MeV
- Ionization caused by triton and proton is collected on an electrode
- 70% of neutrons are absorbed when the product of gas pressure x thickness x neutron wavelength is 16 atm. cm. Å
- Modern detectors are often "position sensitive" – charge division is used to determine where the ionization cloud reached the cathode.



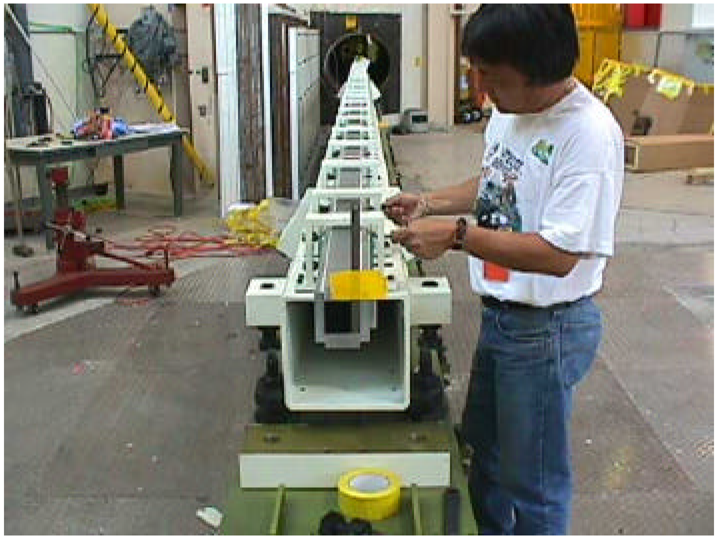
A selection of neutron detectors – thin-walled stainless steel tubes filled with high-pressure ^{3}He.

Essential Components of Modern Neutron Scattering Spectrometers



Horizontally & vertically focusing monochromator (about 15 x 15 cm^2)

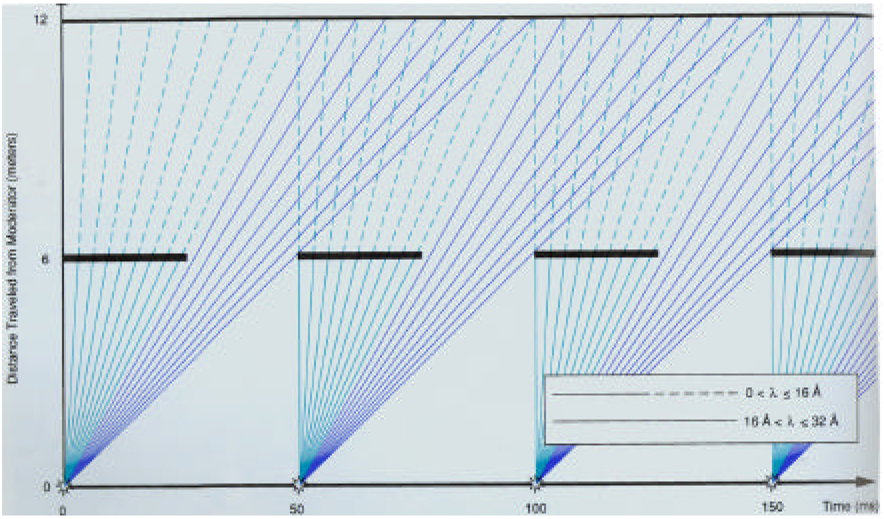
Pixelated detector covering a wide range of scattering angles (vertical & horizontal)



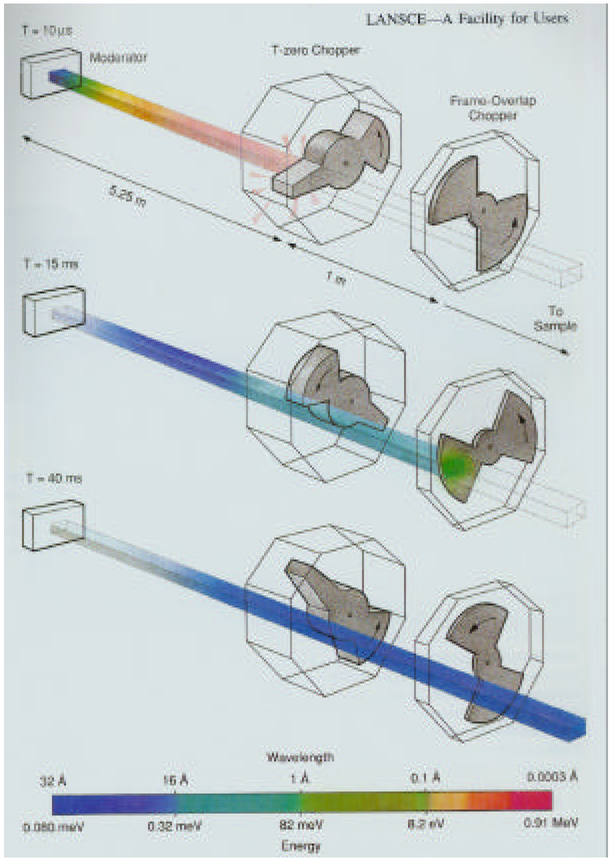
Neutron guide (glass coated either with Ni or “supermirror”)

Rotating Choppers Are Used to Tailor Neutron Pulses at Reactors and Spallation Sources

- T-zero choppers made of Fe-Co are used at spallation sources to absorb the prompt high-energy pulse of neutrons
- Cd is used in frame overlap choppers to absorb slower neutrons



Fast neutrons from one pulse can catch-up with slower neutrons from a succeeding pulse and spoil the measurement if they are not removed.This is called “frame-overlap”



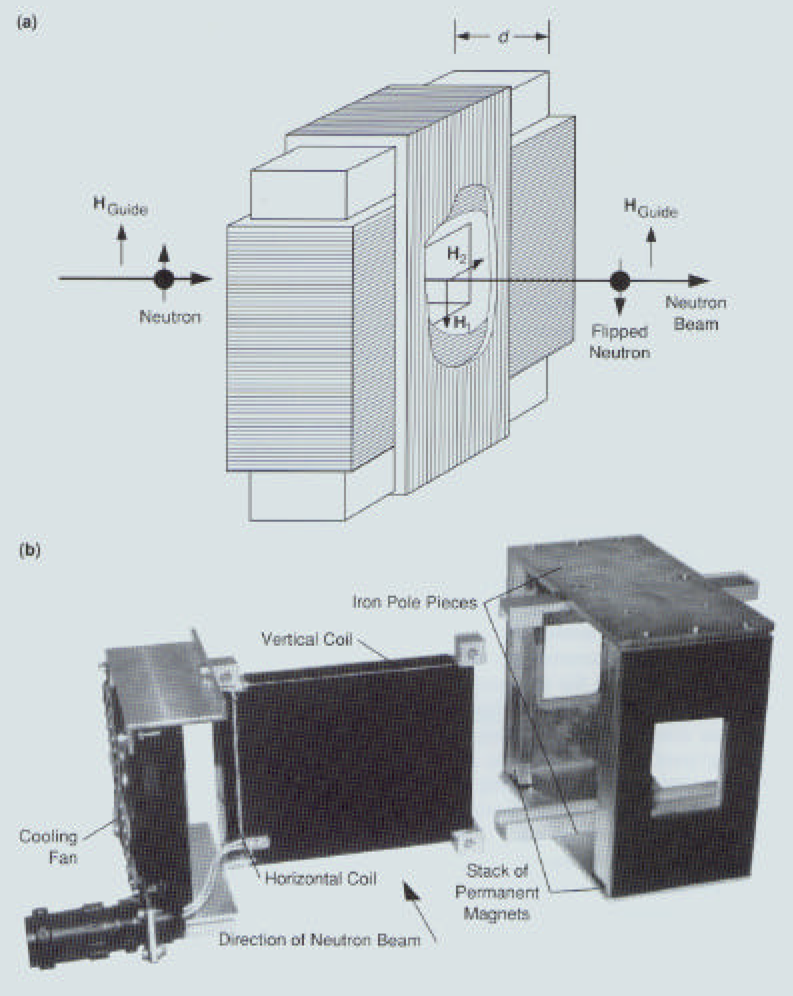
Larmor Precession & Manipulation of the Neutron Spin

- In a magnetic field, H, the neutron spin precesses at a rate

$$u_L = -gH/2p = -2916.4H \ \text{Hz}$$

where γ is the neutron's gyromagnetic ratio & H is in Oesteds

- This effect can be used to manipulate the neutron spin
- A "spin flipper" – which turns the spin through 180 degrees is illustrated
- The spin is usually referred to as "up" when the spin (not the magnetic moment) is parallel to a (weak ~ 10 – 50 Oe) magnetic guide field



Next Lecture

3. Diffraction
    1. Diffraction by a lattice
    2. Single-crystal diffraction and powder diffraction
    3. Use of monochromatic beams and time-of-flight to measure powder diffraction
    4. Rietveld refinement of powder patterns
    5. Examples of science with powder diffraction
        - Refinement of structures of new materials
        - Materials texture
        - Strain measurements
        - Structures at high pressure
        - Microstrain peak broadening
        - Pair distribution functions (PDF)