EUROPEAN
SPALLATION
SOURCE

# Moderators

# Part 1

# Physics elements

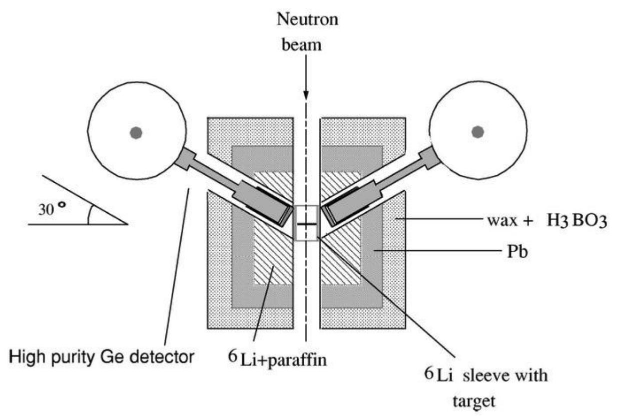
Luca Zanini

V Course "Neutrons for chemistry and Materials Science Applications", Erice, 8 June 2017

# **Worked with neutrons since 1995 at various places**

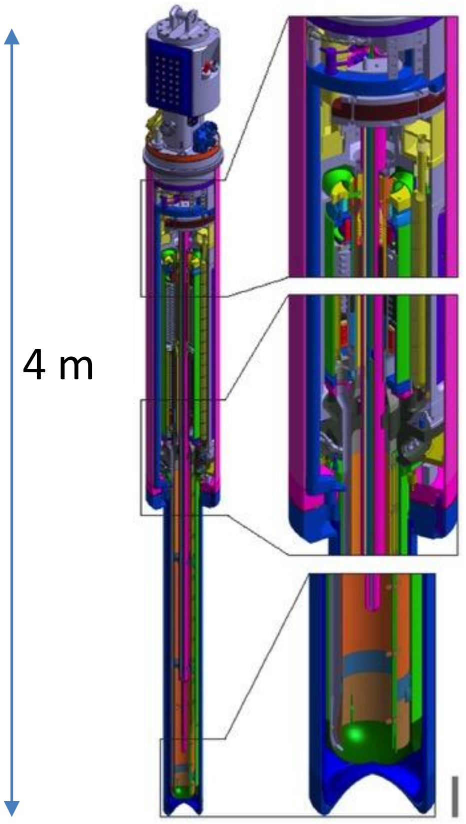
GELINA (IRMM, Belgium) nTOF (CERN) WNR (Los Alamos)
SINQ (PSI, Switzerland) ESS (Sweden)

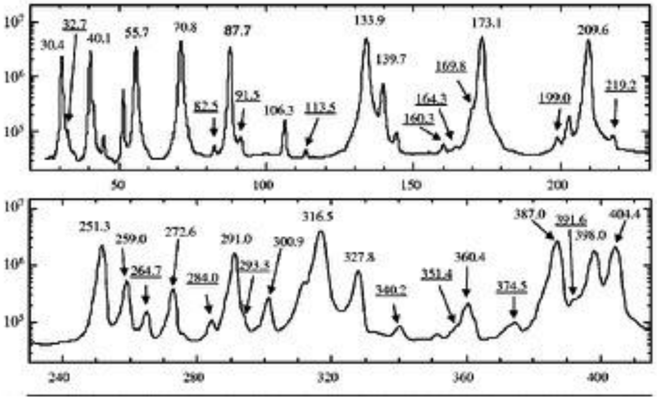
# Background and areas of interest



- ❑ Areas of interest
  - ❑ Neutrons from cold, thermal, resonances, high-energy
    - ❑ Experimental measurements (capture gamma-rays, cross sections,…)
  - ❑ Accelerator driven systems
  - ❑ Spallation target design
  - ❑ Moderator design

MEGAPIE, liquid Pb/Bi target





# Contents

- ☐ Neutron interactions
- ☐ Cross sections
- ☐ Neutron production
- ☐ Slowing down and thermalization
- ☐ Brightness and Liouville theorem

# Neutron

Discovered in 1932 (Chadwick)

Mn=1.67 x $10^{-27}$ kg

Magnetic moment $\mu_n = -1.91\ \mu_N$.

$$\mu_N = \frac{e\hbar}{2m_p}$$

Spin = $\hbar\sqrt{s(s+1)}$, $s$=½ (fermion)

$t_{1/2}$ = 10.2 min

# Types of neutron-nucleus interactions

Elastic scattering

$$n + X \rightarrow n + X$$

In elastic scattering the total kinetic energy of the neutron-nucleus system is conserved.

Inelastic scattering

$$n + X \rightarrow n + X^*$$

change of energy of target nucleus or molecule

Reactions

$$n + X \rightarrow Y + \ \ldots$$

the final constellation is different from the initial one

# Elastic scattering $(n, n)$

$$Z^A + n \rightarrow Z^A + n$$

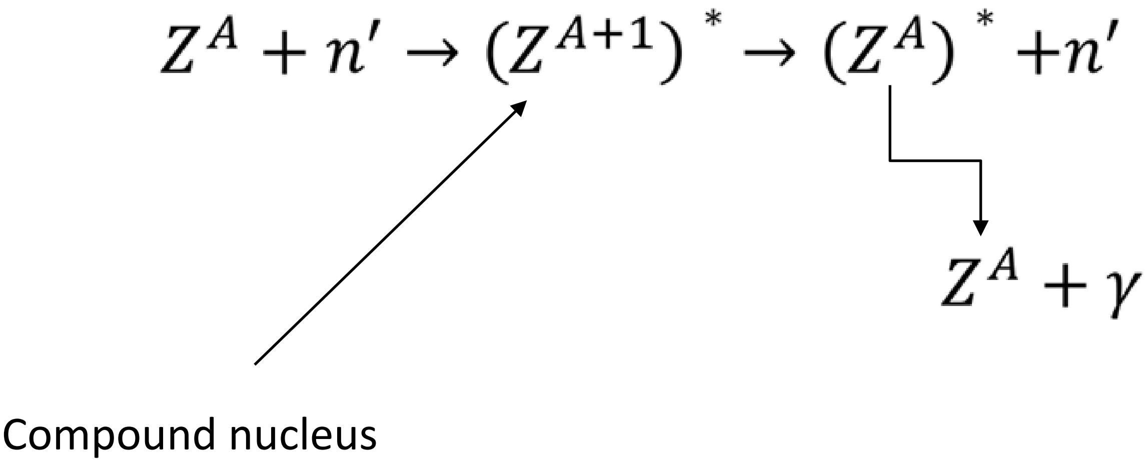
The initial and final constellation are identical and the total kinetic energy of the neutron-nucleus system is conserved.

# Inelastic scattering $(n, n')$

$$Z^A + n' \rightarrow (Z^A)^* + n'$$

The initial and final constellation are identical except that the product nucleus is in an excited state.

The product nucleus in an inelastic-scattering event usually emits one or more gamma rays to reach its ground state.



$$Z^A + n' \rightarrow (Z^{A+1})^* \rightarrow (Z^A)^* + n'$$

$$Z^A + \gamma$$

Compound nucleus

# Example of reactions: radiative capture $(n, \gamma)$

$(n, \gamma)$, radiative capture

$$n + Z^{A} \rightarrow \left(Z^{A+1}\right)^{*} \rightarrow Z^{A+1} + \gamma$$

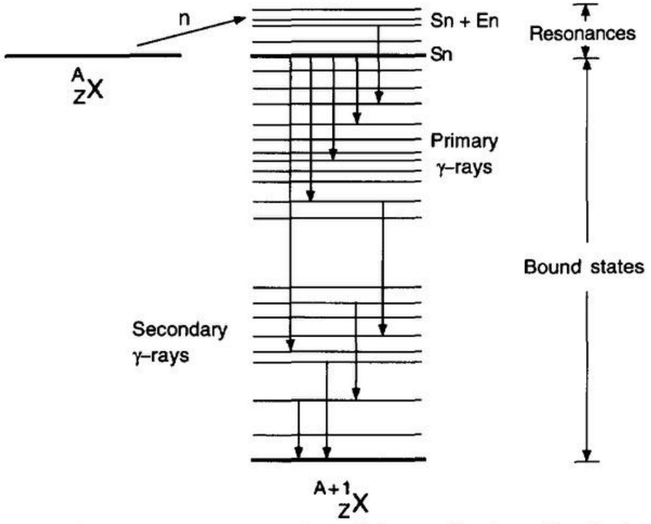


Figure 2.3: Schematic representation of the mechanism of radiative neutron capture. The lines below $S_n$ represent bound states of the compound nucleus, while the upper lines represent resonance states.

# Example of reactions: fission (n,f)

$$n + Z^{A} \rightarrow (Z^{A+1})^{*} \rightarrow Z_1^{A1} + Z_2^{A2}$$

$$Z_1 + Z_2 = Z$$

$$A_1 + A_2 = A$$

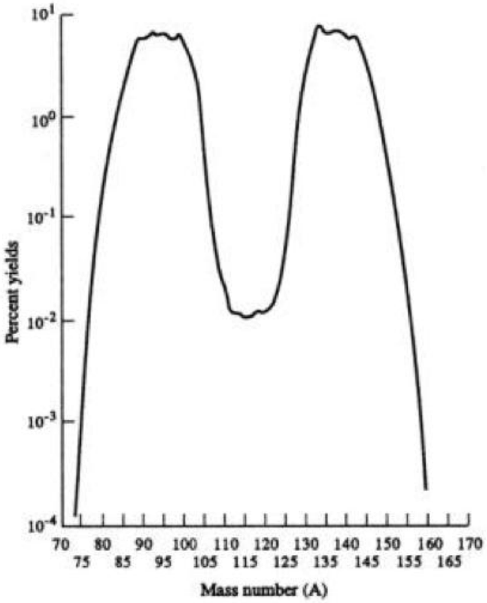


FIG. 6.3 Yield of fission products according to mass number (Courtesy of T. R. England of Los Alamos National Laboratory).

# Cross sections

*Number of j interactions for a flux of A particles* $\phi_a$ *and number per unit volumes* $N_b$ *of particles B:*

$$I_j = \sigma_{ab}^{j} \phi_a N_b$$

# Classification of neutron cross sections

The total neutron cross section can be separated into an elastic scattering cross section and a reaction cross section

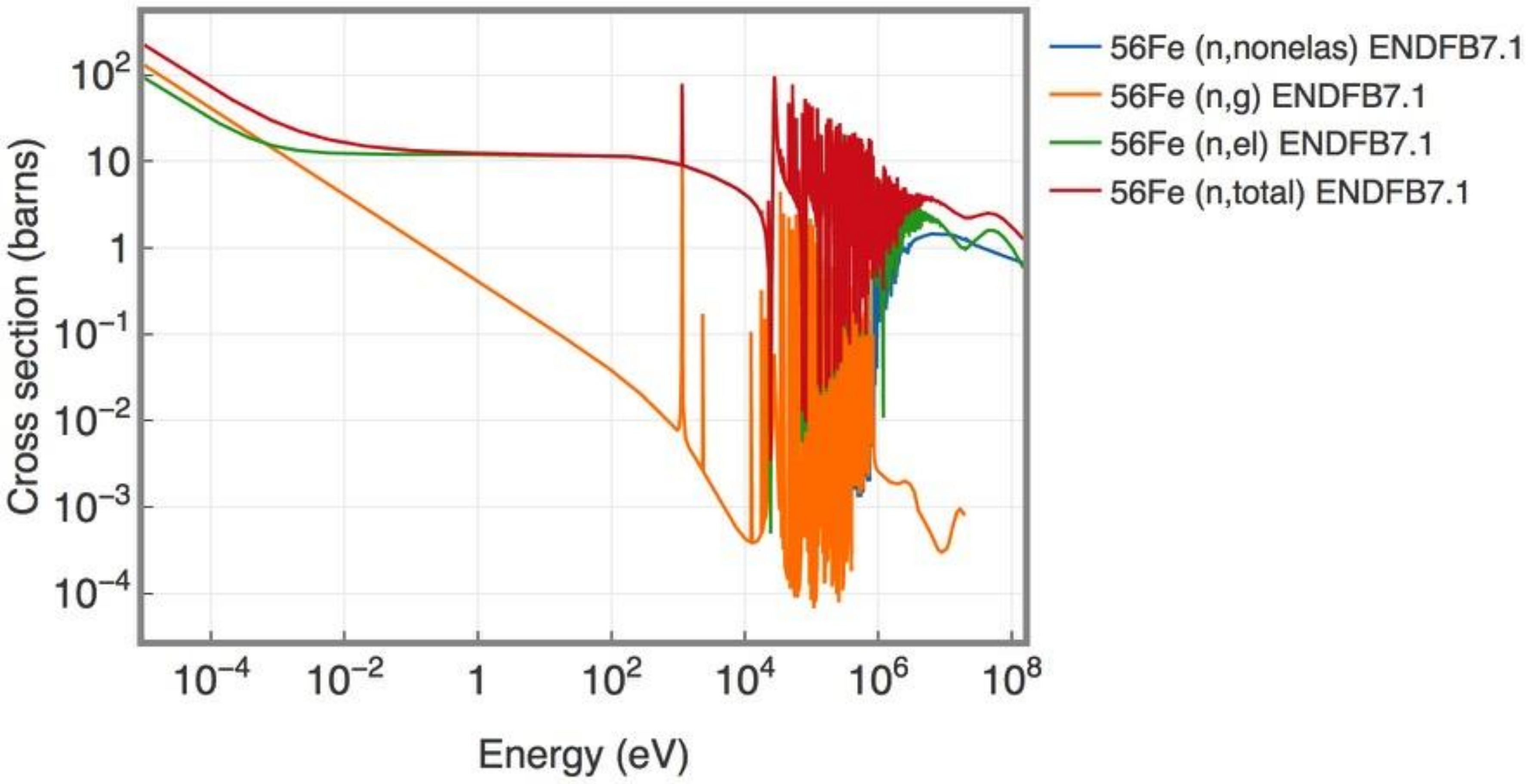
$$\sigma_T = \sigma_n + \sigma_r$$

In elastic scattering the total kinetic energy of the neutron-nucleus system is conserved.

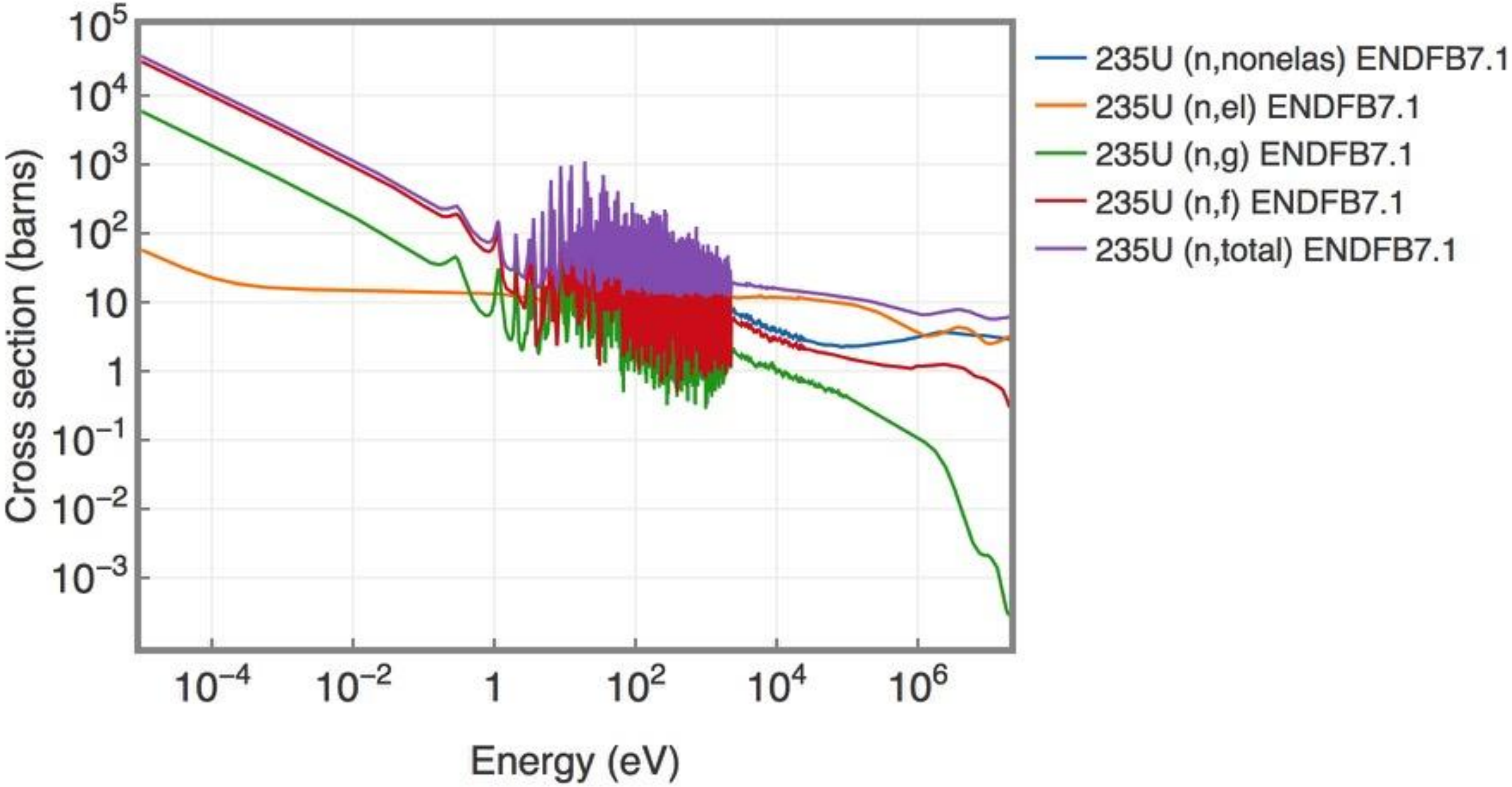
The reaction cross section is the sum of the cross sections for all processes in which the product nucleus is either different from the target nucleus, or is left in an internal energy state different from that of the target nucleus.

e.g. $(n, n')$, $(n, \gamma)$, $(\mathrm{n, p})$, $(\mathrm{n}, \alpha)$, $(n, 2n)$, $(n, f)$.

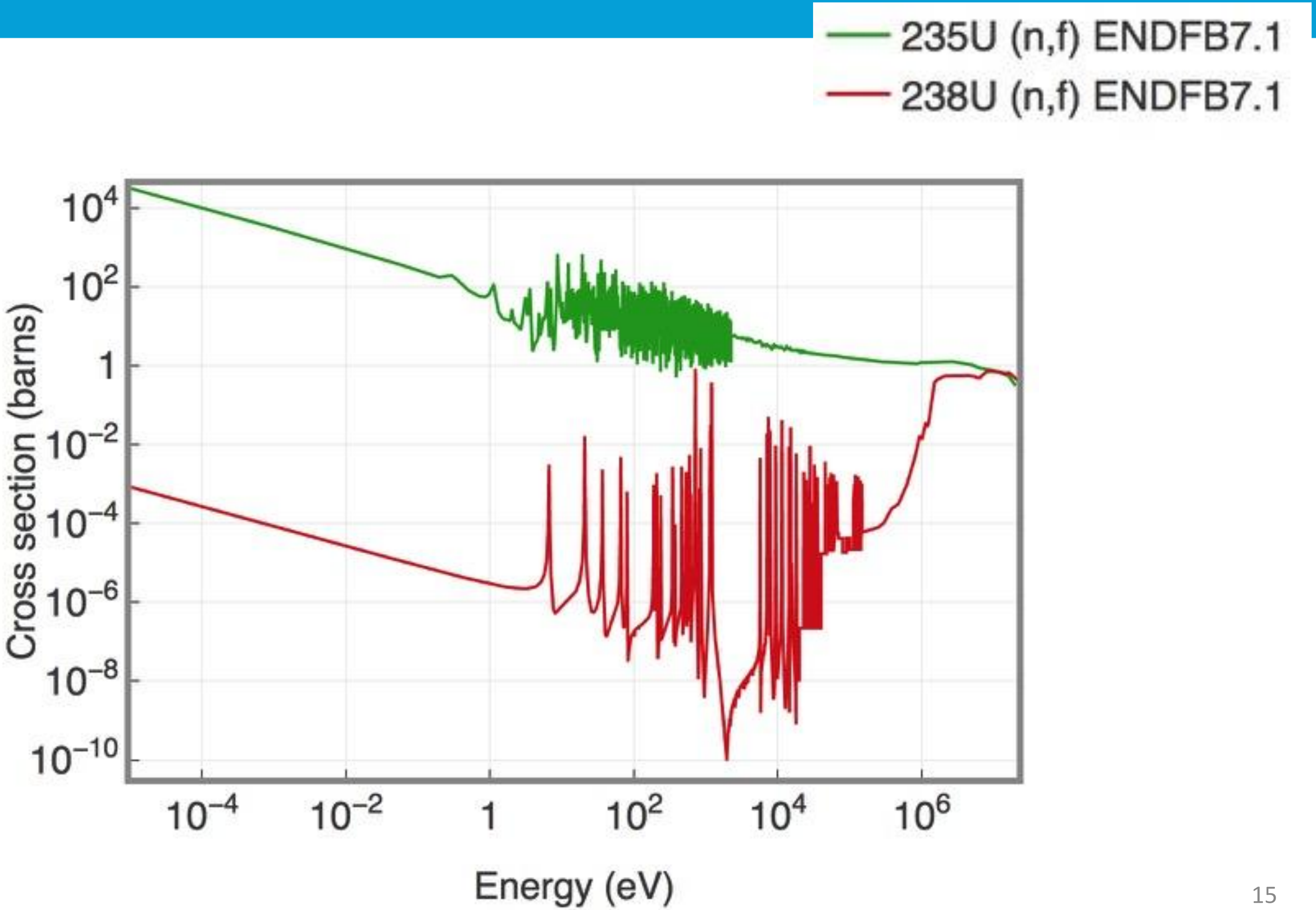
# Examples of cross sections: $^{56}$Fe+n



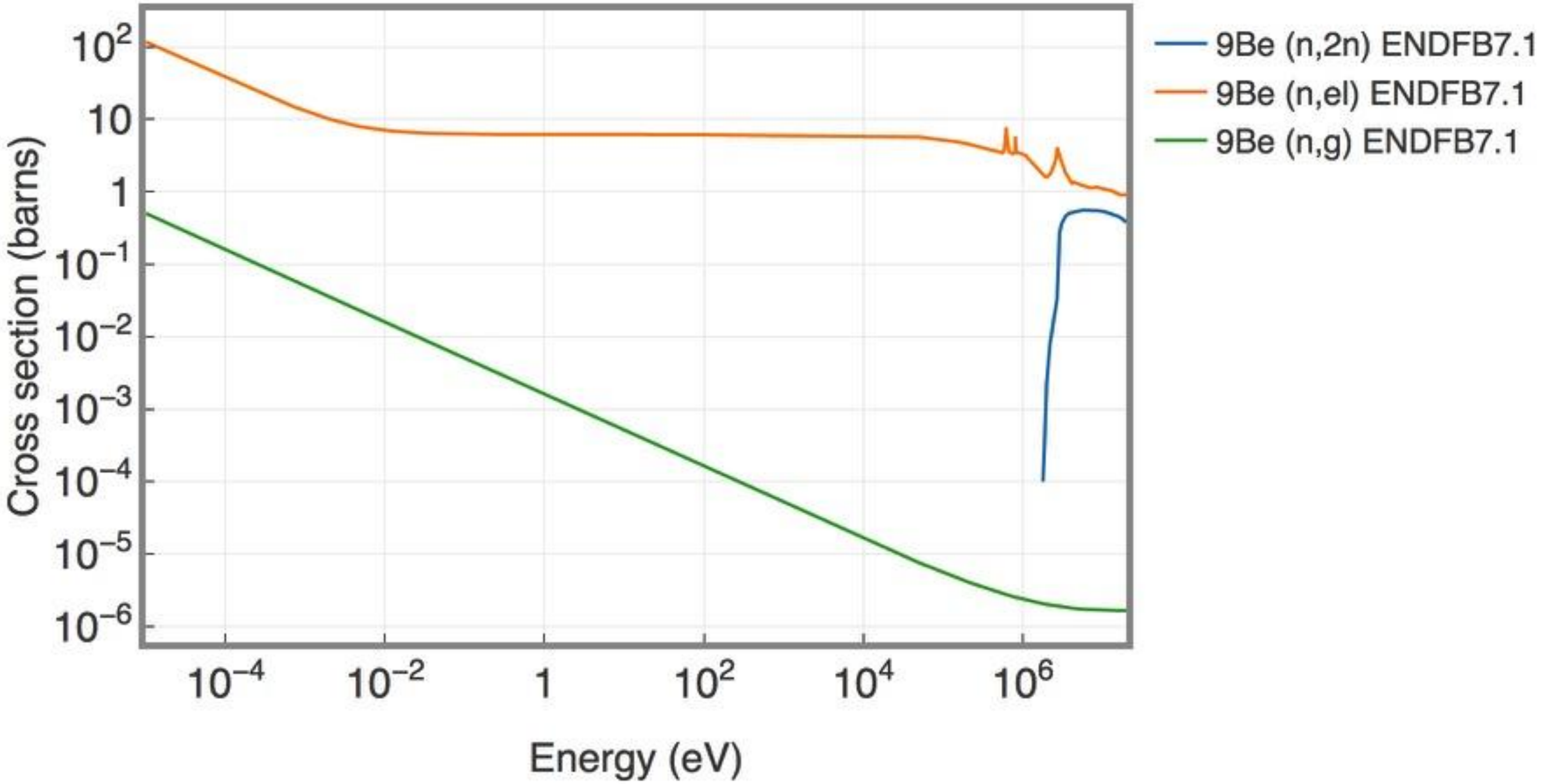
# Examples of cross sections: $^{235}$U+n



# Examples of cross sections: $^{235,238}$U+n



# Examples of cross sections: $^9$Be+n



# Neutron production

**Fast neutrons produced / joule heat deposited in target station**

| | | |
|---|---|---|
| Fission reactors: | $\sim 10^9$ | (in ~ 50 liter volume) |
| Spallation: | $\sim 10^{10}$ | (in ~ 2 liter volume) |
| Fusion:<br>**(but neutron slowing down efficiency reduced by ~20 times)** | $\sim 1.5\text{x}10^{10}$ | (in ~ 2 liter volume) |
| Photo neutrons: | $\sim 10^9$ | (in ~ 0.01 liter volume) |
| Nuclear reaction (p, Be): | $\sim 10^8$ | (in ~ 0.001 liter volume) |
| Laser induced fusion: | $\sim 10^4$ | (in ~ $10^{-9}$ liter volume) |

**Spallation: most favorable for the foreseeable future**

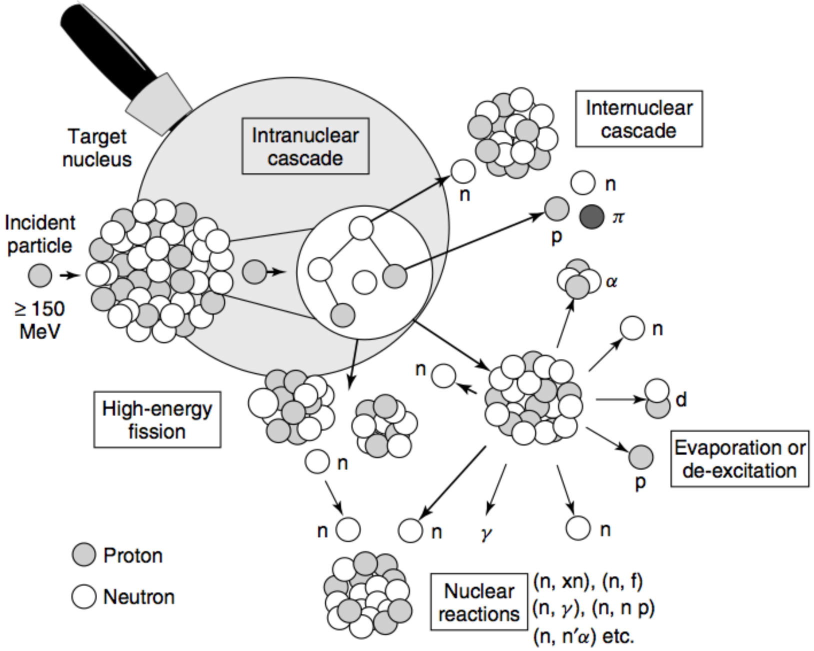
(F. Mezei)

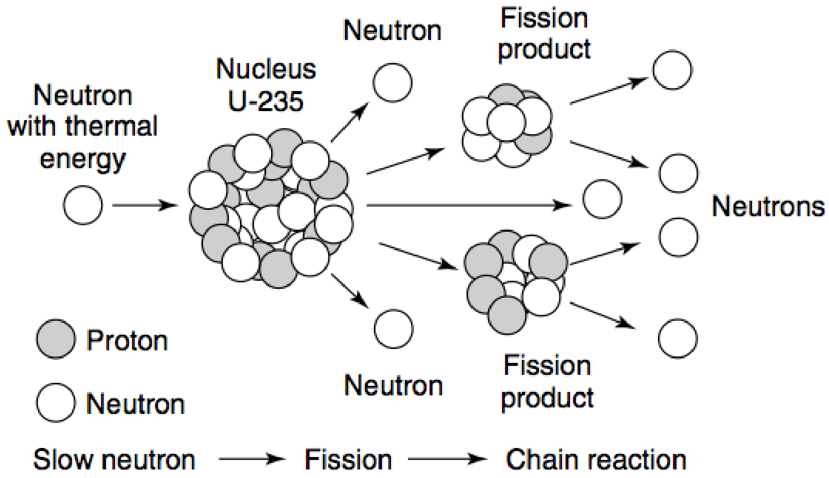
# The spallation process

The term *spallation* refers to a complex of reactions initiated by interaction of high-energy (~ GeV) particles (p, n, π, ...) with heavy nuclei. W. H. Sullivan and G. T. Seaborg coined the term in April, 1947 to describe the phenomenon, whereby the target emits a fairly large number of neutrons in a multiple-collision process.

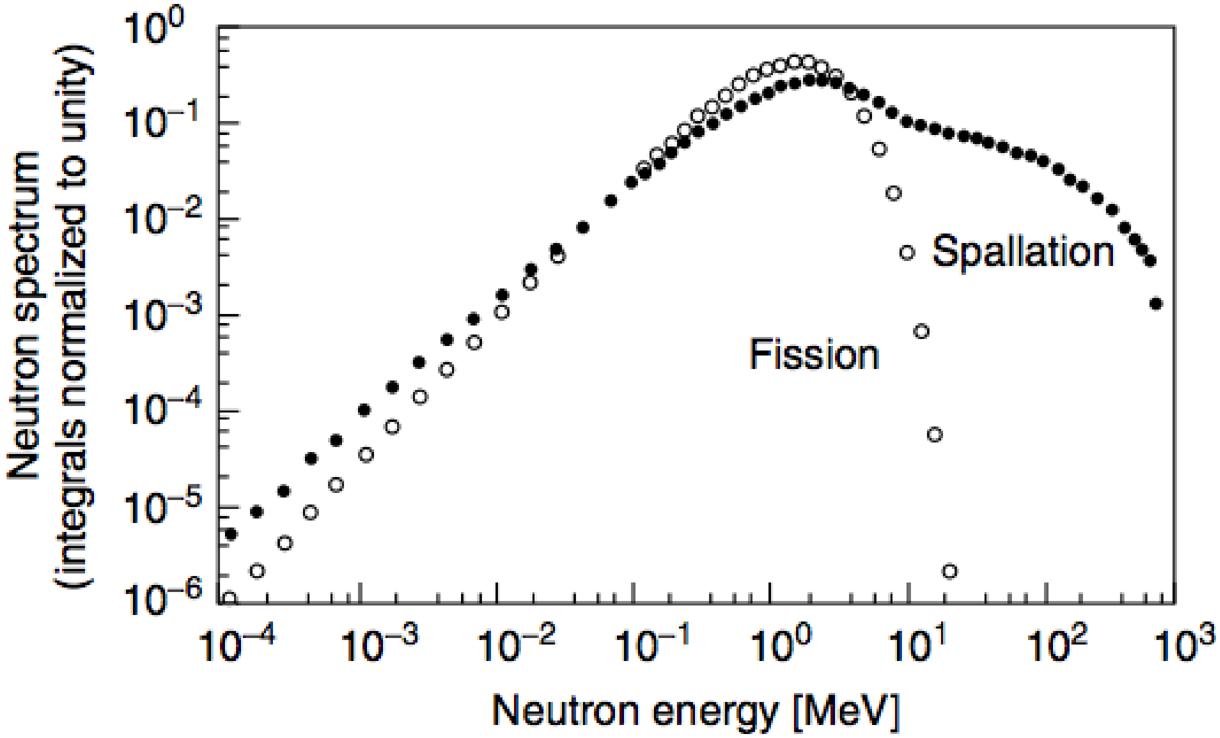
- ☐ Fast Direct Process:
  - ☐ Intra-Nuclear Cascade (nucleon-nucleon collisions)
- ☐ Pre-Compound Stage:
  - ☐ Pre-Equilibrium
  - ☐ Multi-Fragmentation
- ☐ Compound Nuclei:
  - ☐ Evaporation (mostly neutrons)
  - ☐ High-Energy Fissions
- ☐ Inter-Nuclear Cascade
- ☐ Low-Energy Inelastic Reactions
  - ☐ (n,xn)
  - ☐ (n,nf)
  - ☐ etc...

In contrast to fission, spallation cannot be self sustaining!



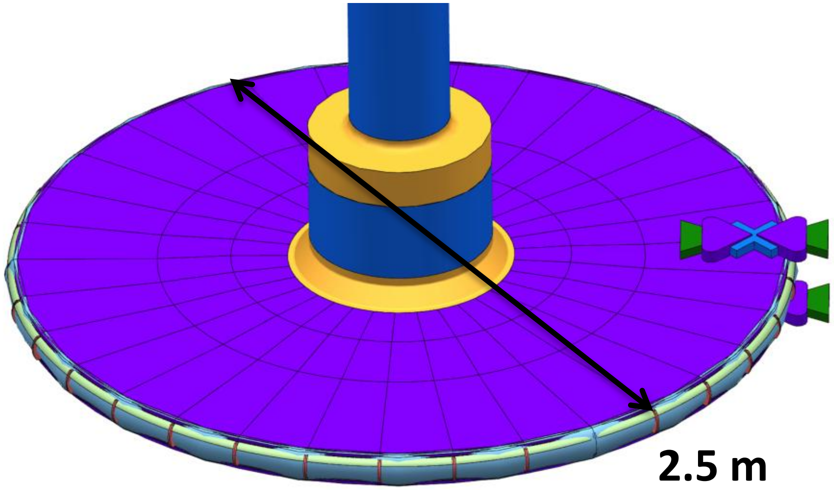


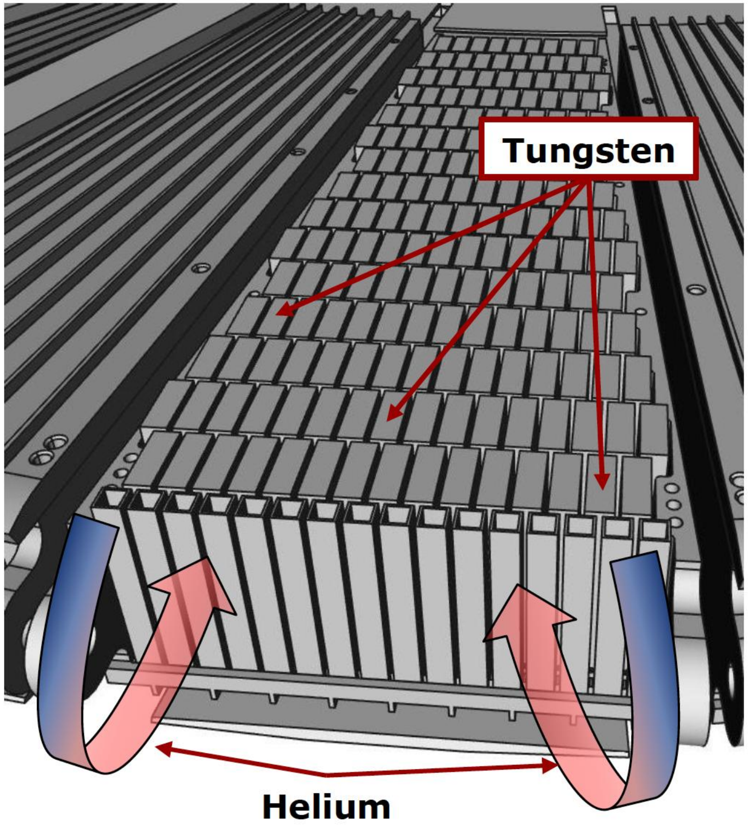
# Neutron energy spectra: fission vs spallation



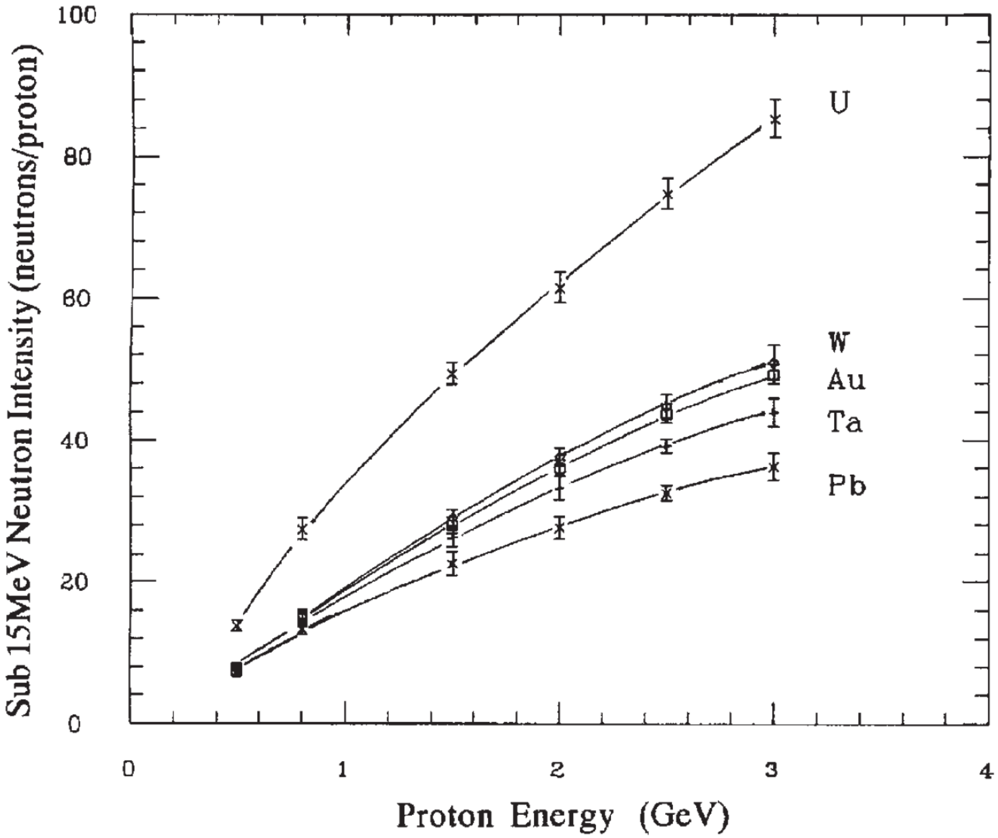
In any case, steady or pulsed, reactor or accelerator, the primary reactions produce most of their neutrons at energies of a few MeV. This is far too high an energy to be useful for slow-neutron scattering. Therefore in slow-neutron scattering facilities there are *moderators* arranged around the primary source to slow down the source neutrons to useful energies.

# ESS spallation target: 5 MW (2 GeV, 2.5 mA) proton beam on tungsten target





# Neutron yield for different targets and energies



$$Y(E) = a(A + 20)(E_{\mathrm{GeV}} - b) \quad (0.2 \leqslant 1.5\,\mathrm{GeV})$$

a=0.1 (0.19 for $^{238}$U), b=0.12 GeV

# Spallation vs fission

- No criticality issues
- No actinide waste
- Proliferation safe
- Advantage by exploiting time structure
- Less heat per neutron than other nuclear processes
- High degree of design flexibility

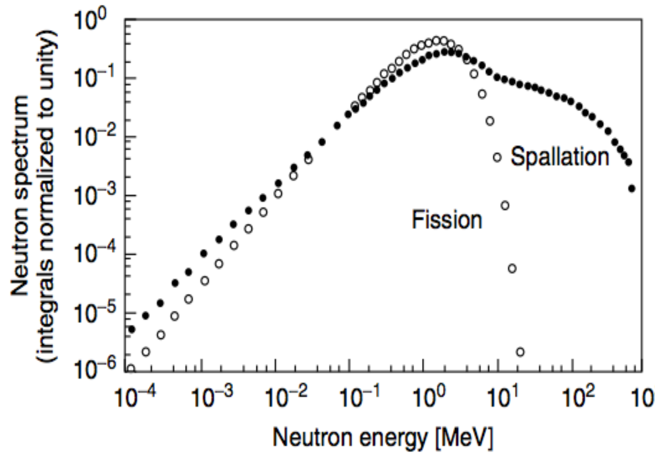
BUT

- Demanding shielding issues
- Extra complexity by need of accelerator
- More distributed radioactivity (e.g. in cooling loops and shielding)

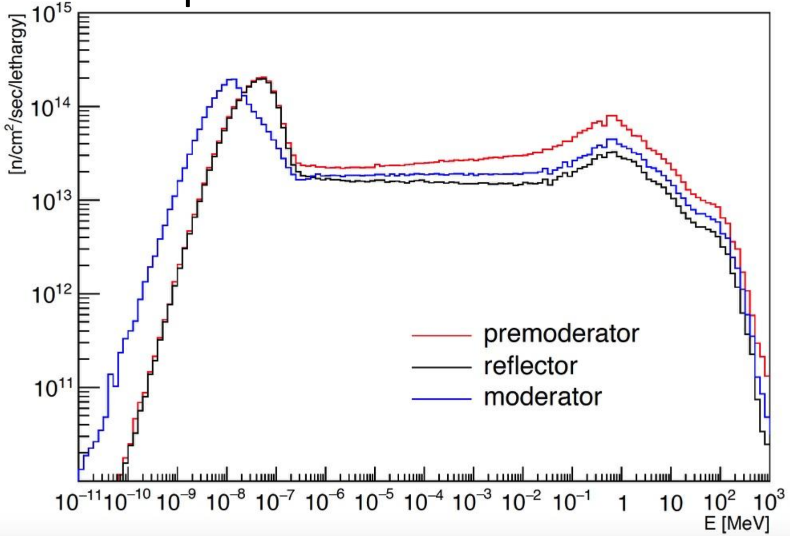
(G. Bauer)

# From spallation neutrons (MeV) to thermalization (meV)

- ☐ Spallation
  - ☐ Neutron leakage from target
- ☐ Slowing down and thermalization in premoderator and moderator
- ☐ Reflection in reflectors



Spectra inside ESS moderators



# Slowing down

- In the slowing-down region the spectrum is approximately proportional to 1/E ; more exactly, $(1/E)^{1-\alpha}$, where E is the neutron energy and α a small number between 0.1 and 0.2 determined by the neutron leakage from the moderator during the slowing-down.

- We can assume in the neutron-nucleus interaction that the nucleus is at rest and “free”
- Inelastic scattering results in excitation of the nucleus

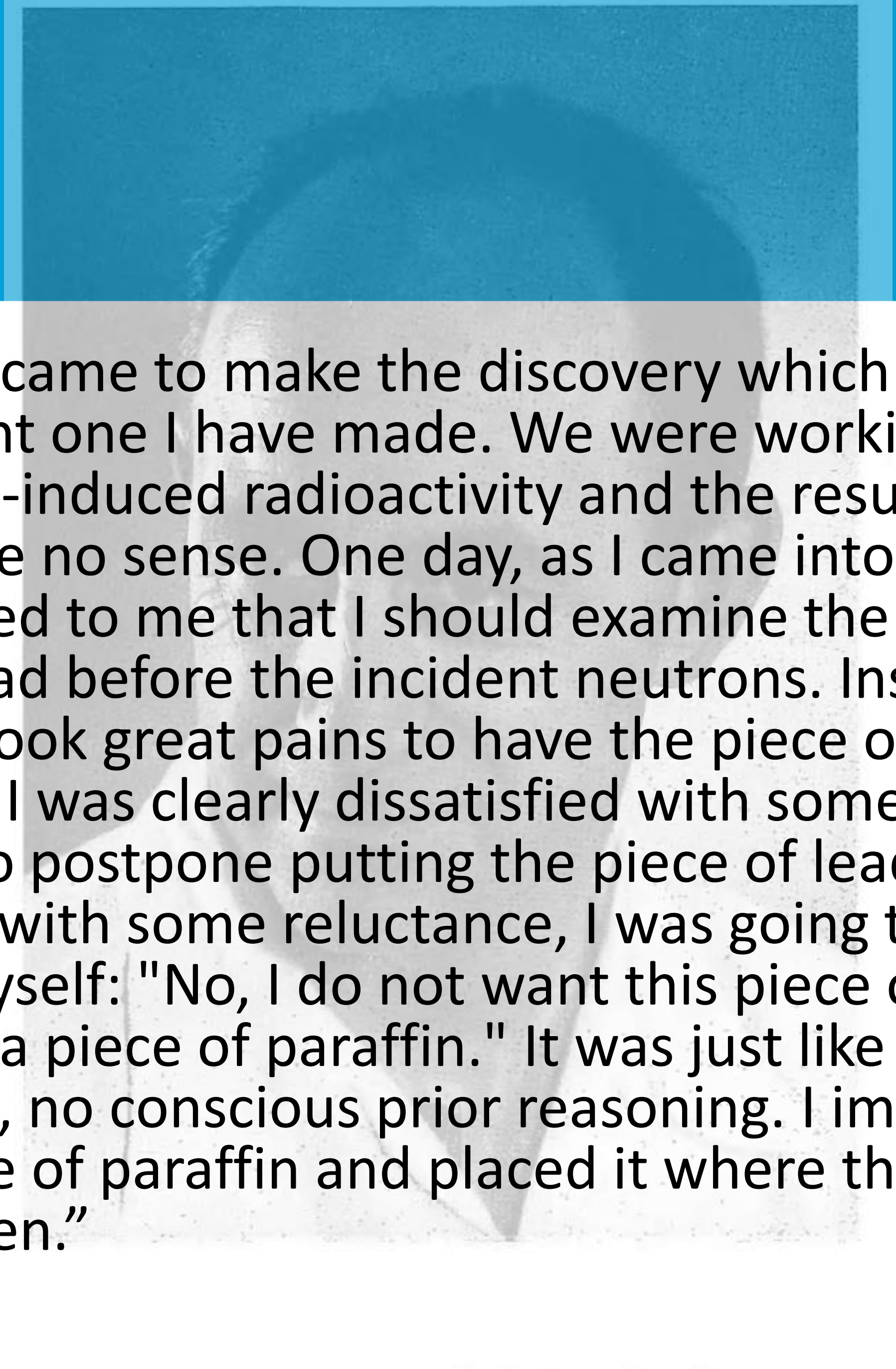
# Thermalization

- In the thermal equilibrium region, the spectrum exhibits a Maxwellian distribution due to the detailed balance between neutrons and scattering atoms.

- The nucleus cannot be considered at rest
- It cannot be considered free
- Neutrons can decrease or increase energy
- Inelastic scattering results in change of the internal energy of the molecule or crystal
  - It can give gain or loss of energy to the neutron

# Thermalization

- In 1935 Fermi discovered in Rome that some materials irradiated in water bath activated much more than when exposed to bare neutron sources.
- He reasoned that neutrons colliding with protons in water slowed down and were captured with higher probability.



“I will tell you how I came to make the discovery which I suppose is the most important one I have made. We were working very hard on the neutron-induced radioactivity and the results we were obtaining made no sense. One day, as I came into the laboratory, it occurred to me that I should examine the effect of placing a piece of lead before the incident neutrons. Instead of my usual custom, I took great pains to have the piece of lead precisely machined. I was clearly dissatisfied with something: I tried every excuse to postpone putting the piece of lead in its place. When finally, with some reluctance, I was going to put it in its place, I said to myself: "No, I do not want this piece of lead here; what I want is a piece of paraffin." It was just like that with no advance warning, no conscious prior reasoning. I immediately took some odd piece of paraffin and placed it where the piece of lead was to have been.”

E. FERMI – *Los Alamos*, 1946.

The extraordinary result of substituting paraffin wax for a heavy element like lead was a dramatic increase in the intensity of the activation. "About noon," Segre’ remembers, "everybody was summoned to watch the miraculous effects of the filtration by paraffin. At first I thought a counter had gone wrong, because such strong activities had not appeared before, but it was immediately demonstrated that the strong activation resulted from the filtering by the paraffin of the radiation that produced the radioactivity."

Laura Fermi says "the halls of the physics building resounded with loud exclamations: 'Fantastic! Incredible! Black magic!'"

Not even his most important discovery kept Fermi from going home for lunch. (…) He pondered in solitude and may have considered the difference between wood and marble tables as well as between paraffin and lead. When he returned in mid afternoon he proposed an answer: the neutrons were colliding with the hydrogen nuclei in the paraffin and the wood. That slowed them down. Everyone had assumed that faster neutrons were better for nuclear bombardment because faster protons and alpha particles always had been better. But the analogy ignored the neutron's distinctive neutrality. A charged particle needed energy to push through the nucleus' electrical barrier. A neutron did not. Slowing down a neutron gave it more time in the vicinity of the nucleus, and that gave it more time to be captured.

They went home to dinner but met afterward at Amaldi's, whose wife had a typewriter, to prepare a first report. "Fermi dictated while I wrote," Segre' remembers. "He stood by me; Rasetti, Amaldi, and Pontecorvo paced the room excitedly, all making comments at the same time." Laura Fermi recreates the scene: "They shouted their suggestions so loudly, they argued so heatedly about what to say and how to say it, they paced the floor in such audible agitation, they left the Amaldis' house in such a state, that the Amaldis' maid timidly inquired whether the guests had all been drunk."

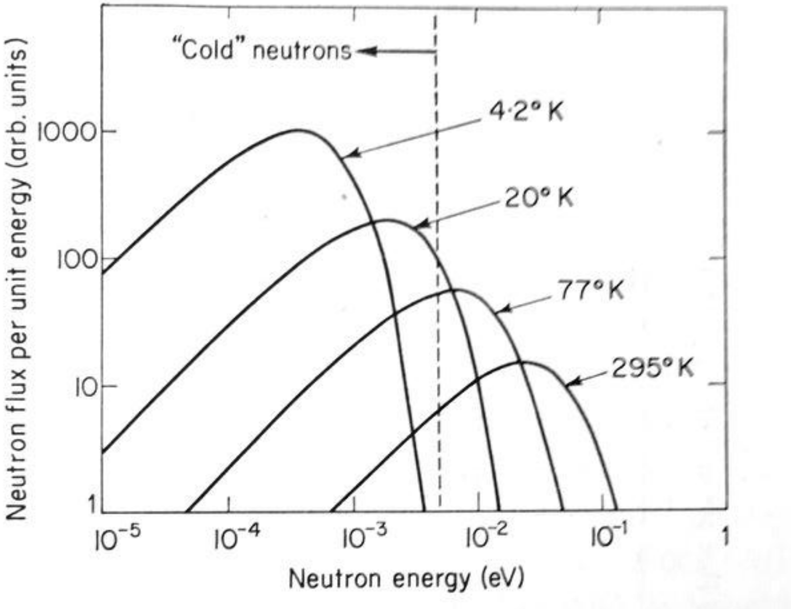
*(From R. Rhodes, The making of the atomic bomb)*

# Maxwell-Boltzmann distribution

*Perfect gas, no absorption*

$$n_f(E)dE = 2n_F \frac{E}{(kT)^2} e^{-\frac{E}{kT}} dE$$

T=293.15 K, kT=0.0253 eV,
v=2200 m/s

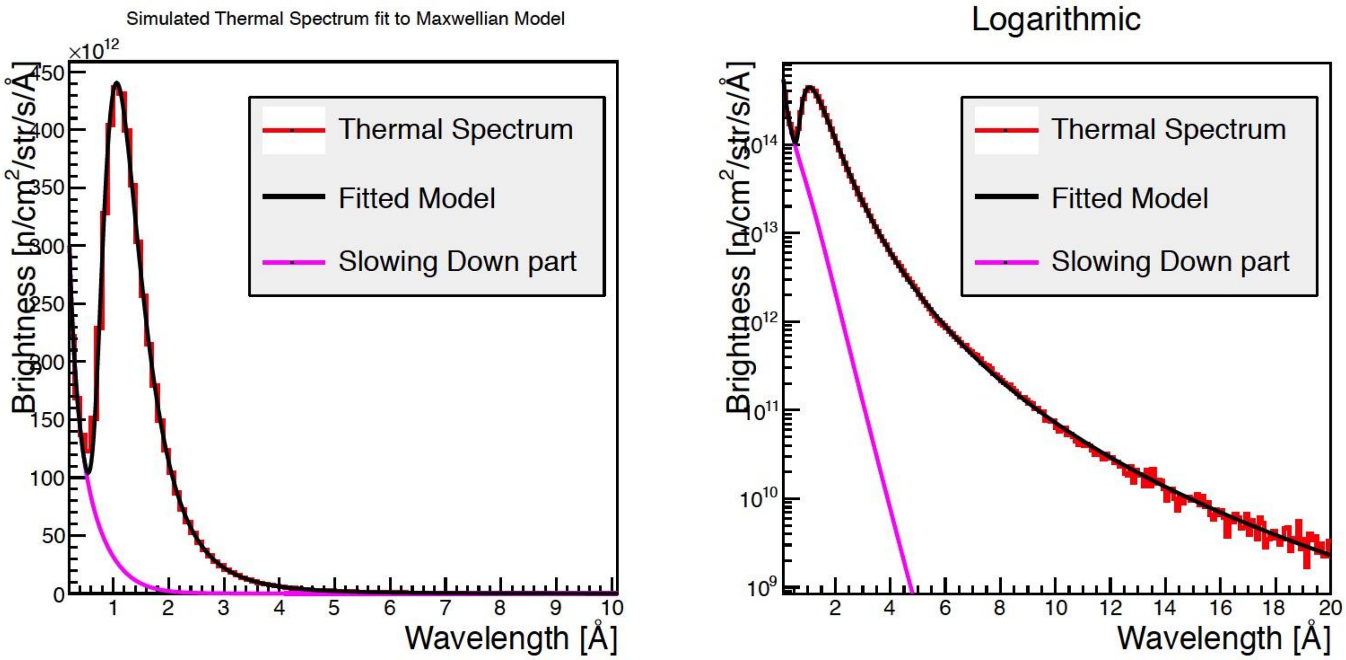


Maxwell distributions at boiling
points of nitrogen, hydrogen and helium

# Slowing down + Maxwellian describe the neutron spectrum in water

$$S_{Th}(\lambda) = I_{Th}\frac{2k_{Th}^2}{T^2\lambda^5}e^{-\frac{k_{Th}}{T\lambda^2}} + I_{SD}\frac{1}{\lambda}\frac{1}{1+e^{\alpha(\lambda-\lambda_{cf})}}$$

Fit of ESS thermal moderator spectrum (Schoenfeldt, ICANS XXI)



# Interactions in the chemical region

The slowing down of neutrons below a few eV needs special consideration because in this energy region the following phenomena will play a role:

(a) the thermal agitation of the atoms of the moderator (Doppler effect);

(b) the chemical forces binding these atoms in crystals or molecules and the quantization of the corresponding vibrational and rotational levels;

(c) the interference between waves scattered from various atoms of the same crystal or molecule.

(b) and (c) are phenomena associated with the structure of the material of the moderator. They would not occur in a monoatomic gas.

# Interactions in the chemical region

Because of the quantization of the vibrational and rotational degrees of freedom a sharp distinction can be made between elastic and inelastic collisions;

- elastic collisions are those which leave the target molecule or crystal in its initial state *i* and the neutron with energy unchanged.
- Inelastic collisions, on the contrary, take place with an energy exchange between neutron and molecule or crystal; if the molecule is excited to a higher state the neutron loses energy; if the molecule is deexcited i.e., if it undergoes a transition from a higher to a lower level, the neutron energy is correspondingly increased.

Inelastic scattering in the chemical region is different from the high-energy region. At high energy is a nuclear phenomenon, where the neutron is absorbed to form a compound nucleus. In the chemical region it is associated with the bonds between the struck nucleus and the molecule or crystal of which the nucleus is a part.

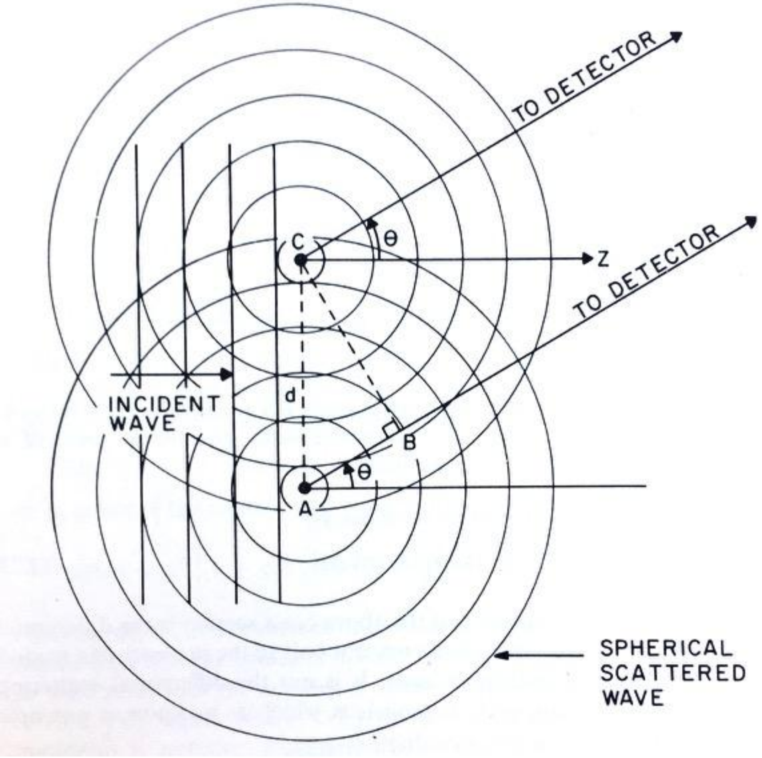
# Coherent scattering

Neutrons with energies in the chemical region have de Broglie wavelengths of the order of the interatomic spacings in molecules and solids (a few Angstrom units)

$$\lambda = \frac{h}{\sqrt{2m_n E}} = \frac{0.287\ \text{Å}}{\sqrt{E\ (eV)}}$$

Coherent effects caused by interference among the waves scattered from the various nuclei of the same crystal or molecule arise.

- These effects occur only between waves that describe neutrons with the same energy and spin state.
- Scattered waves add coherently
- Coherent scattering affects only the angular distribution of the scattered neutrons. Neutrons are conserved in scattering.



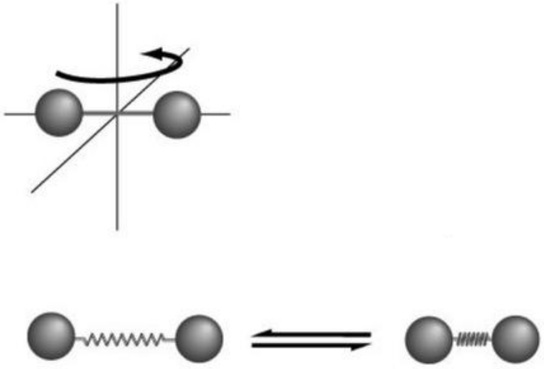
# Energy levels in molecules: vibrational and rotational

Vibrational and rotational levels in molecules are strongly affected by neutron collisions.

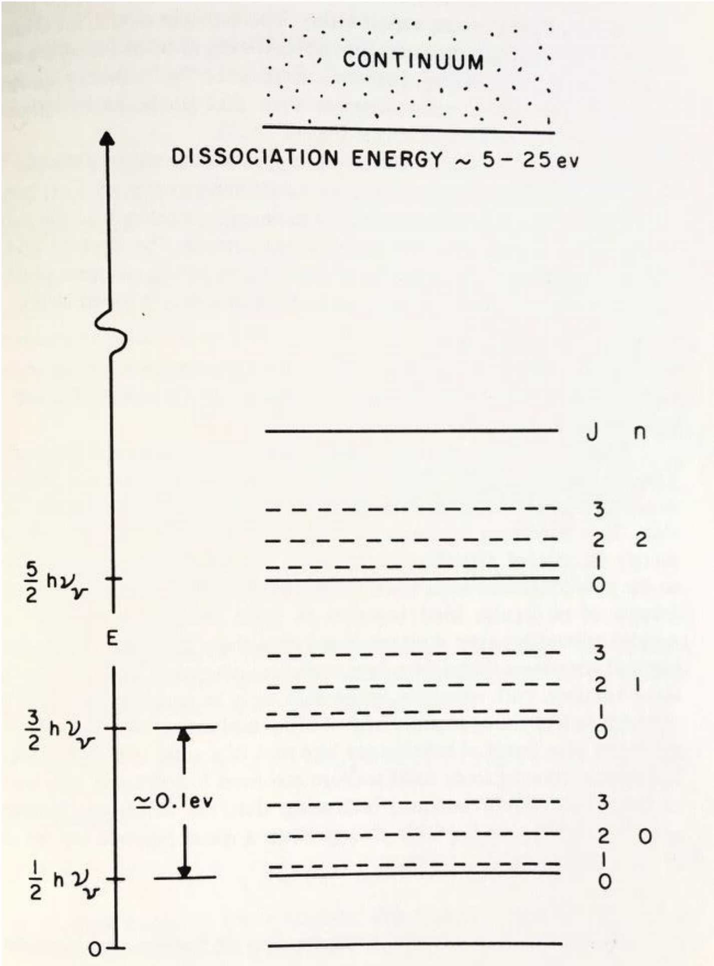
Diatomic molecules such as $H_2$ can rotate as a whole about an axis passing through the center of mass perpendicular to the nuclear axis, and the atoms in the molecule can vibrate relative to one another along the internuclear axis.

Vibrational states have distance of about 100 meV (too much for cold neutrons)

Rotational states have distance of about 10 meV: good for cold neutrons.



Schematic diagram of vibration-rotation energy levels in a diatomic molecule



# Properties of $H_2$

Hydrogen exists in two forms, ortho- and para-$H_2$.
In the ortho form, the proton spins are aligned and the molecule has spin S = 1.

Spin triplet S=1

$$|\uparrow\uparrow\rangle$$

$$|\downarrow\downarrow\rangle$$

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

In the para form, the proton spins are anti-aligned and the molecule has spin S = 0.
Spin singlet S=0

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

At liquid hydrogen temperature (20 K) the parahydrogen ratio at equilibrium is 99.8%.

# Rotational levels of $H_2$ molecule

Quantum mechanically, the rotational states of the free hydrogen molecule are given by

$$\epsilon = \frac{h^2}{Ma^2} J(J+1)$$
$$= 0.015 \frac{J(J+1)}{2} eV$$

Where M is the proton mass and *a* the distance between the protons which is 0.75 Å.

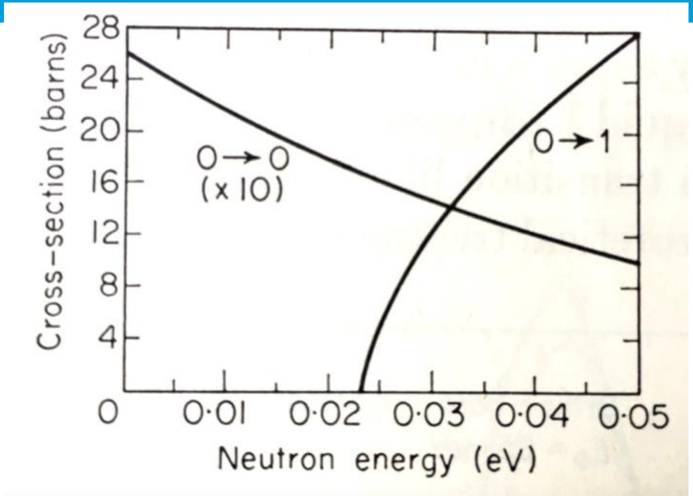
Even values of the quantum number J correspond to the para state and odd values to the ortho state.

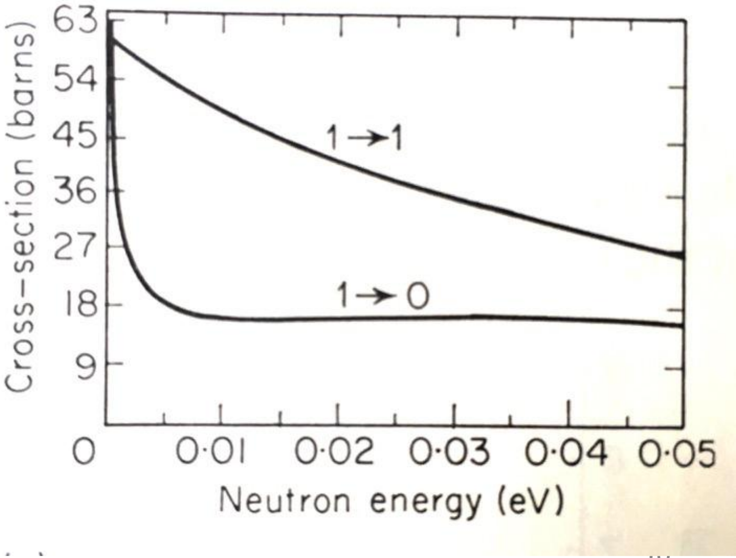
| J | | $\epsilon$ (eV) |
|---|---|---|
| para | ortho | |
| 0 | | 0 |
| | 1 | 0.015 |
| 2 | | 0.045 |
| | 3 | 0.090 |
| 4 | | 0.150 |

# $H_2$ cross sections for neutrons with E < 50 meV

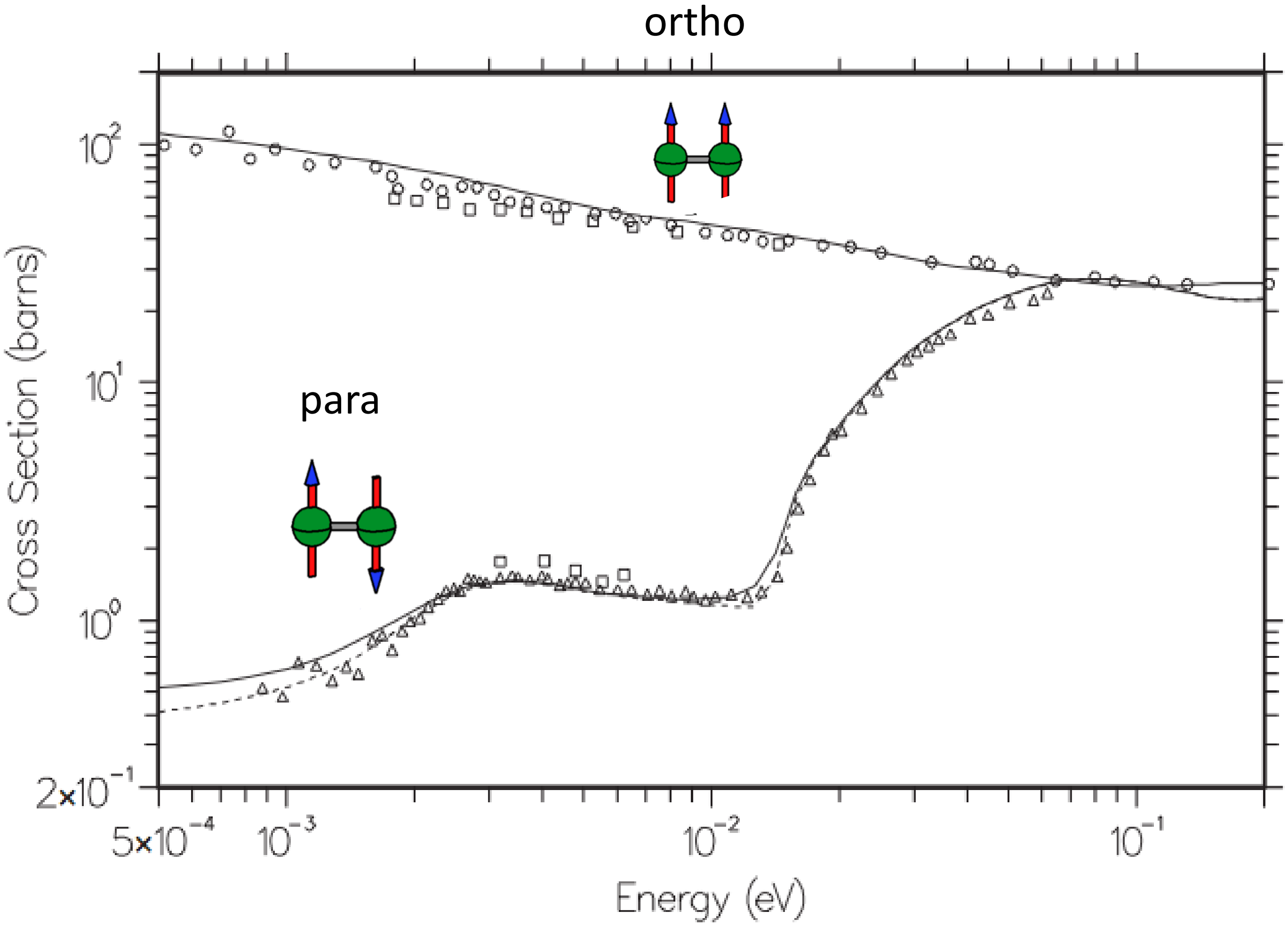
Only J=1 excitations are possible:

$$0 \rightarrow 0\ para - para\ (elastic\ scattering)$$
$$0 \rightarrow 1\ para - ortho\ (inelastic\ scattering)$$
$$0 \rightarrow 0\ ortho\ - ortho\ (elastic\ scattering)$$
$$1 \rightarrow 0\ ortho - para\ (inelastic\ scattering)$$

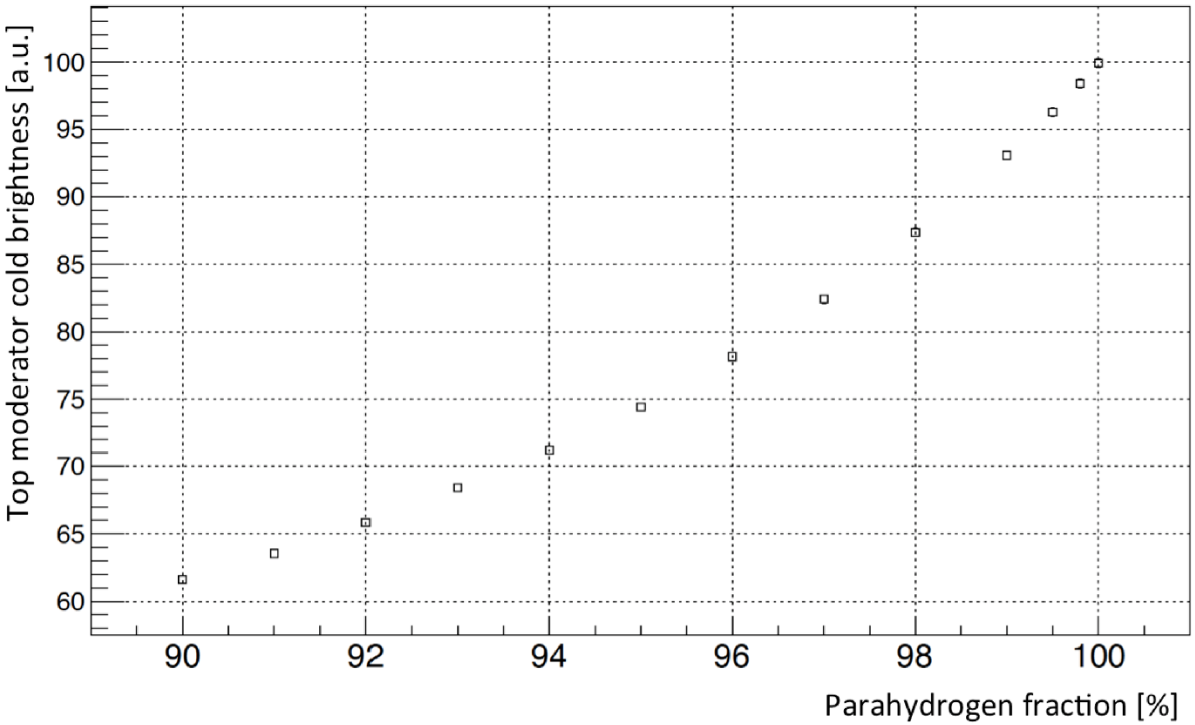




# The resulting cross section is extremely important for moderator design



# Pure parahydrogen is needed to avoid loss in performance



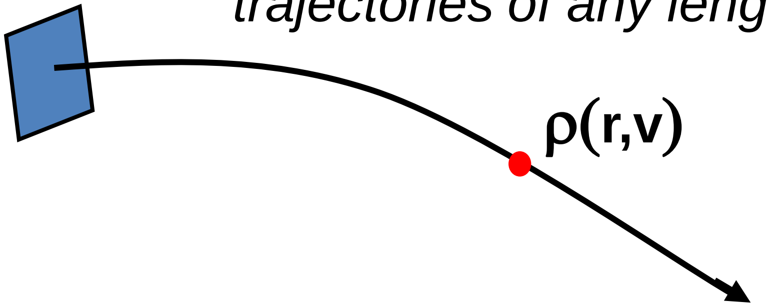
(for 3 cm thick $H_2$ “flat” moderator)

# Reflector neutronics

- The function of a reflector is to enhance slow-neutron intensities by reflecting leakage-neutrons from the target, which do not directly enter the moderator, towards the moderator.
- As reflector materials those having a large macroscopic scattering cross-section such as $D_2O$, Be, graphite (C), iron (Fe), copper (Cu), nickel (Ni), W, Pb, etc, can be considered.
- Reflector materials are classified into two categories, moderating and non-moderating ones.
- Be is a typical moderating reflector material, while Pb is a typical non-moderating one.

# Liouville’s theorem

*Phase space density $\rho$ is constant along particle trajectories of any length in conservative force fields*



*Absolute intensity:*

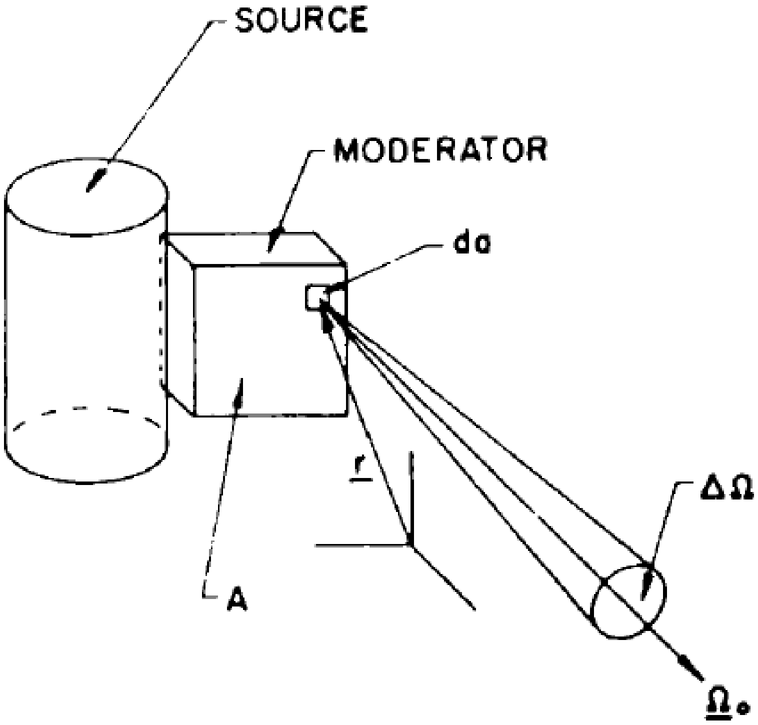
at any point along the beam

$$\phi(\lambda) = \eta\ \phi(\lambda)_{\text{source}}$$

source brightness

(absorption) loss factor ≤ 1

# Liouville's theorem



The Brightness *B* is the product of the speed v times the neutron angular density

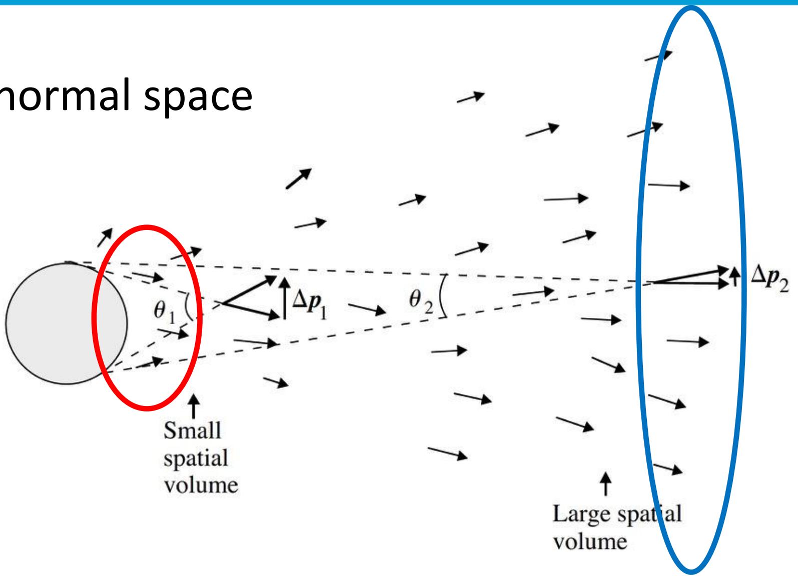
$$B(r,\Omega,E,t) = v\,\frac{n(r,\Omega,E,t)}{dV\,d\Omega dE}$$

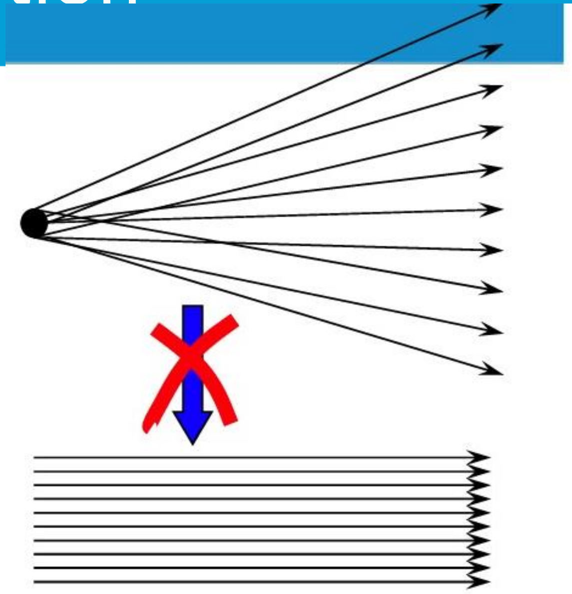
The phase space density ρ is the number of particles in the phase space volume dqdp= $dVp^2dpd\ \Omega$ at time t:

$$\rho(\boldsymbol{q},\boldsymbol{p},t) = \frac{n(\boldsymbol{r},\Omega,E,t)}{dVp^2dpd\Omega} = \frac{v}{p^2}\,\frac{n(\boldsymbol{r},\Omega,E,t)}{dV\,d\Omega dE}$$

# Focusing increases divergence.
# Higher flux, loss in angular resolution

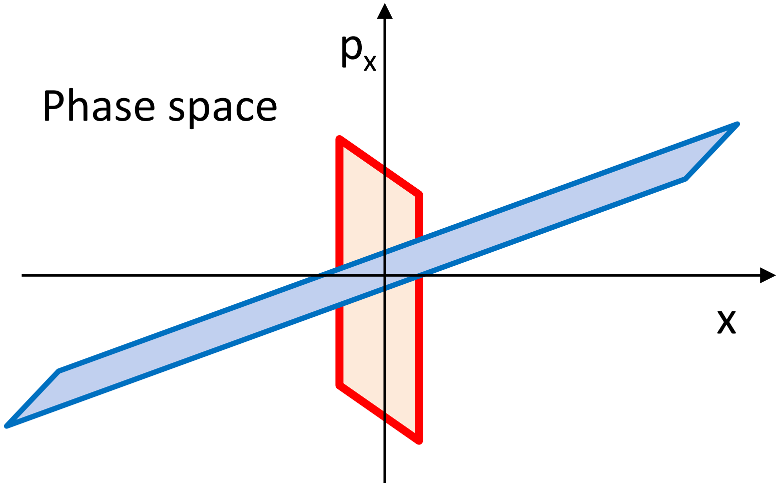
normal space

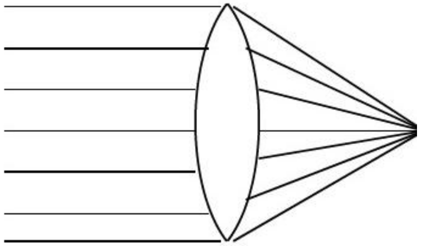




(“no free lunch”)

Phase space



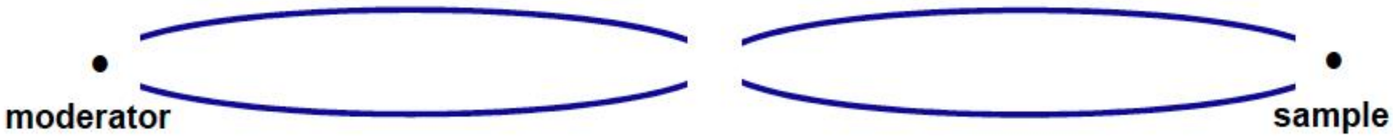


# Importance of Liouville's theorem

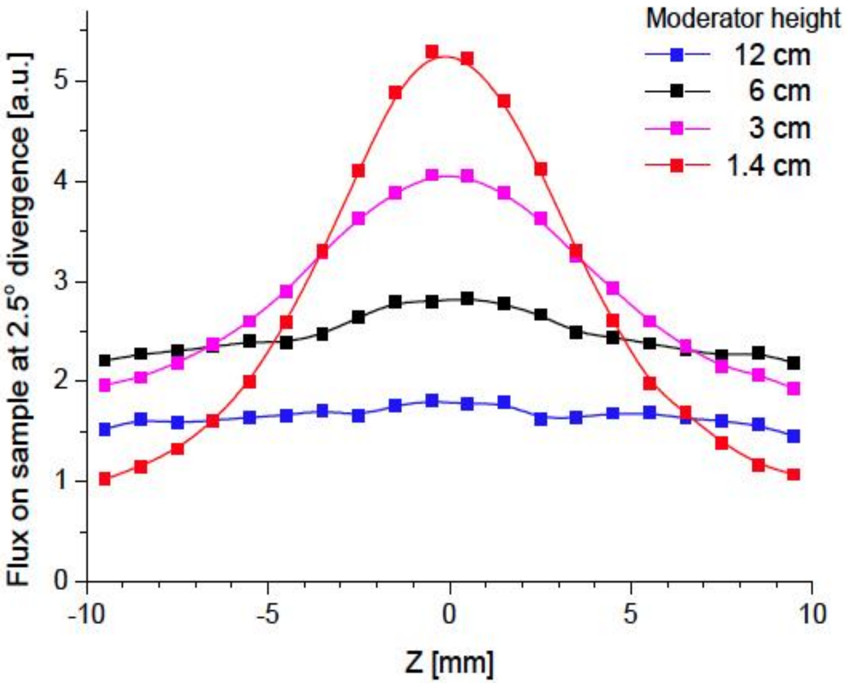
- It links the performance of the moderator to the number of neutrons with desired energy and divergence that reach the sample,
- therefore identifying the brightness as the figure of merit for moderator design.
- It links the work of source and instrument designers

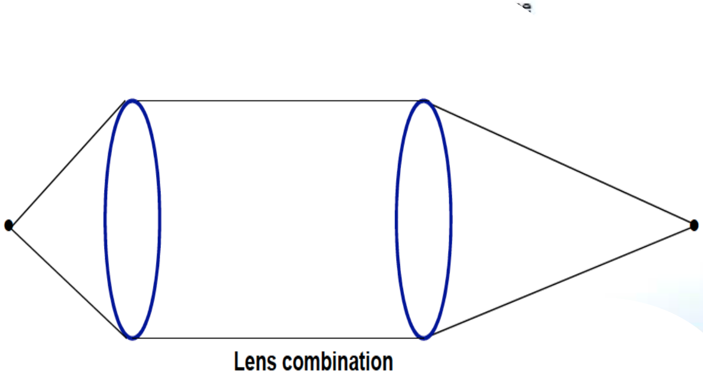
# Flux at sample for different moderator heights

- **Using best proposed / tested supermirror optics**



**Example: 2.5° beam divergence at 80 m**





(F. Mezei)

# Moderators

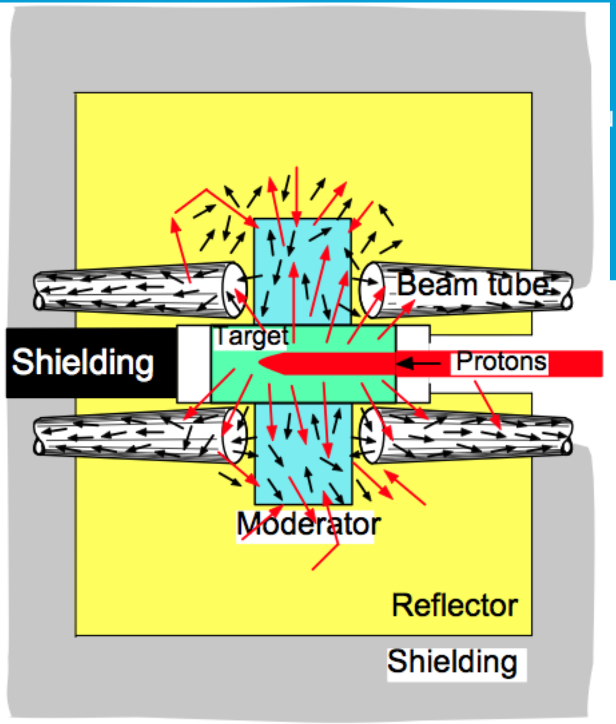
## Part 2

## Existing moderators and moderator design

# Contents

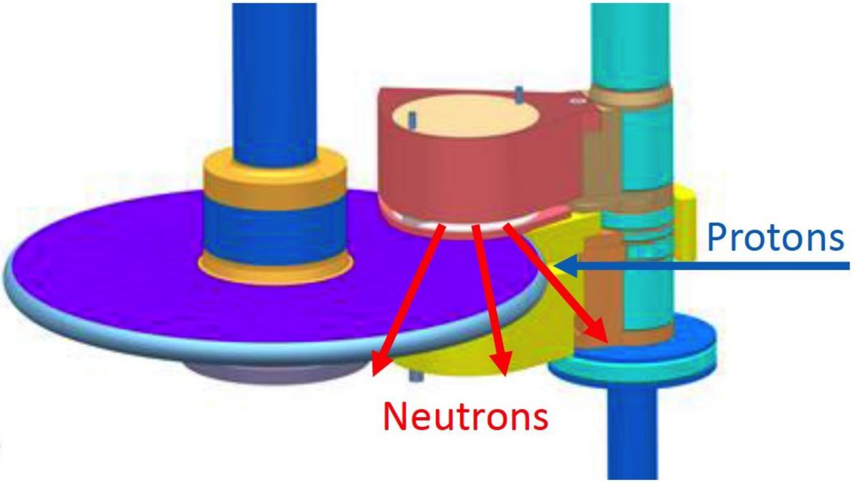
- Principals of moderator design
- Moderators for short pulses and long pulses
- Coupled, decoupled, poisoned moderators
- Design of moderators from holistic approach (from protons on target to neutrons on sample), the case of ESS
- Future possibilities

# Target-moderator-reflector arrangement



The function of a moderator is to convert leakage-neutrons from a target to slow-neutrons with an energy spectrum and pulse characteristics required for experiments.

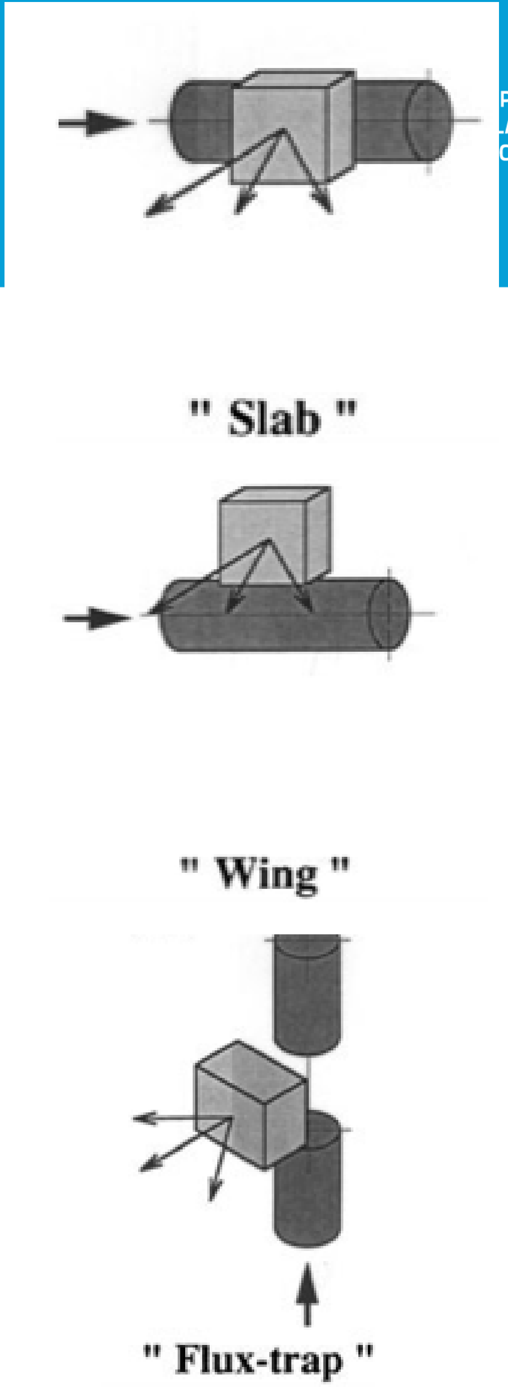
The reflector serves to enhance the neutron output from the moderator at minimum adverse effect on the time structure



An ideal moderating material used for spallation neutron sources should have the following nuclear properties:

- large scattering cross section
- small absorption cross section
- large energy loss per collision.

# Moderators arrangement



- A moderator in the slab geometry can provide higher slow-neutron intensity than the others due to a larger solid angle between the target and the moderator. However, fast and high-energy neutrons leaking into the slow-neutron beam are about a thousand times higher than the other cases. Therefore, direct beam use is almost impossible in spite of its higher slow-neutron intensity.
- The wing-geometry has been most widely used in existing sources, since no instrument views the target directly
- The flux trap geometry is useful for vertical proton beam injection onto the target. The target is divided into two sections along the proton beam axis and moderators are located around the void space between the two target sections.

# Highest flux short pulse sources

SNS (Oak Ridge, USA)

J-PARC (Tokai Japan)

**Instantaneous power on target** (e.g. 1 MW at 60 Hz, i.e. 17 kj in ~1 μs pulses on target): **17 x**

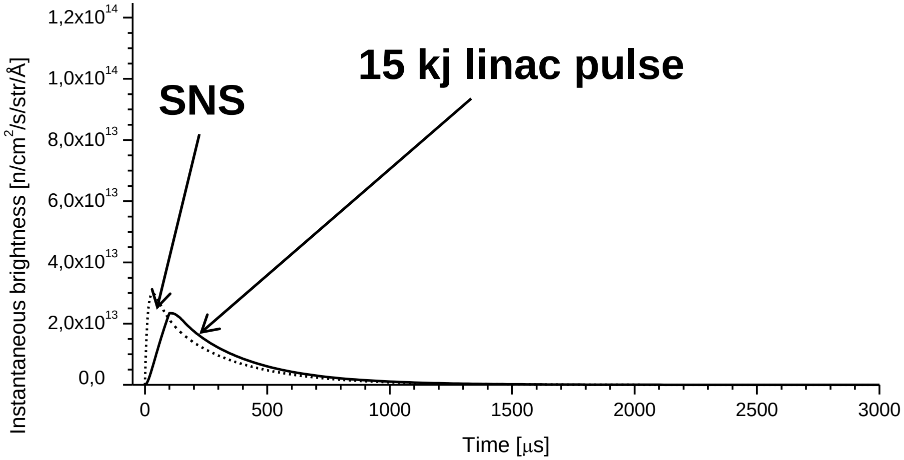
→ **Pressure wave: 300 bar**

Reaches limits of technology

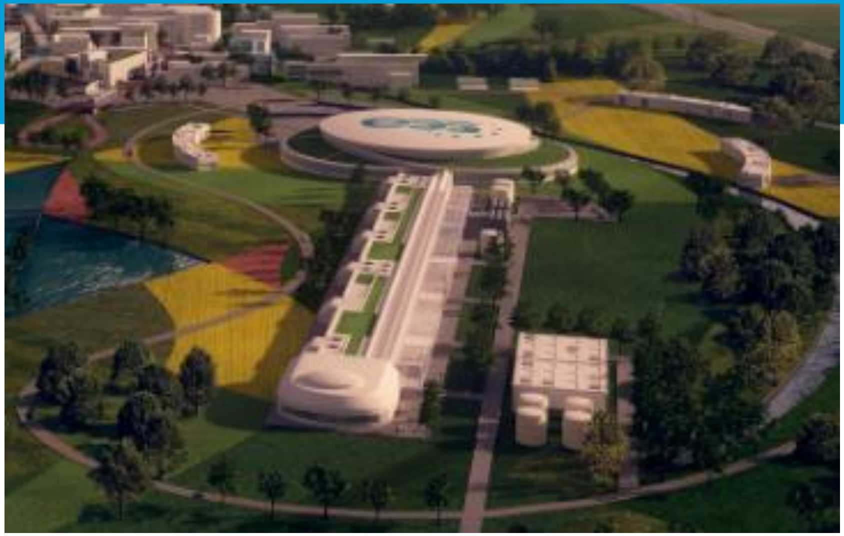
(F. Mezei)

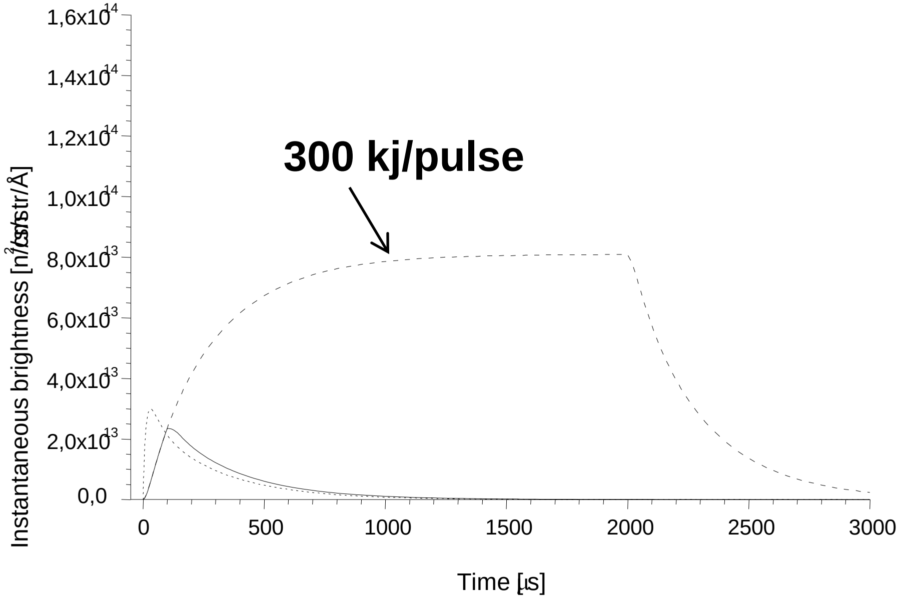
# Highest flux short pulse sources

**But:**
Cost equivalent linear accelerator alone can produce the same **cold neutron pulses by ~100 μs proton pulses at ~ 0.15 GW instantaneous power: 2 x ILL**



# long pulses

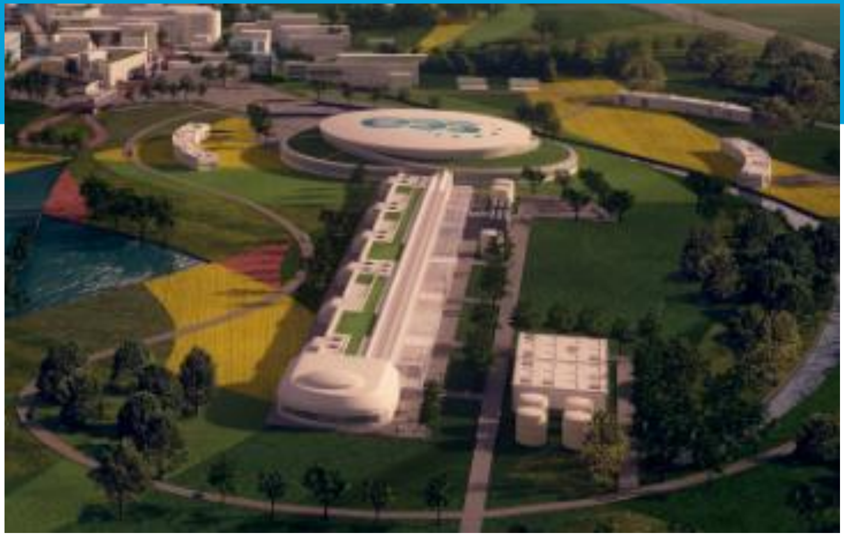


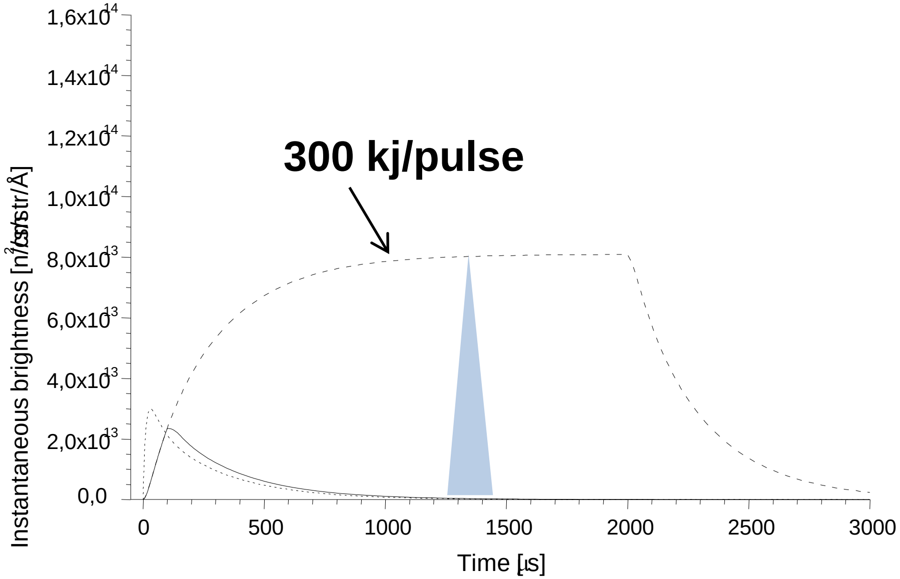


**300 kj/pulse**

Cost equivalent linear accelerator alone can produce the same cold neutron pulses **by ~100 µs proton pulses at ~ 0.15 GW instantaneous power** → Leave the linac on for **more neutrons per pulse and higher peak brightness…**

# long pulse sources

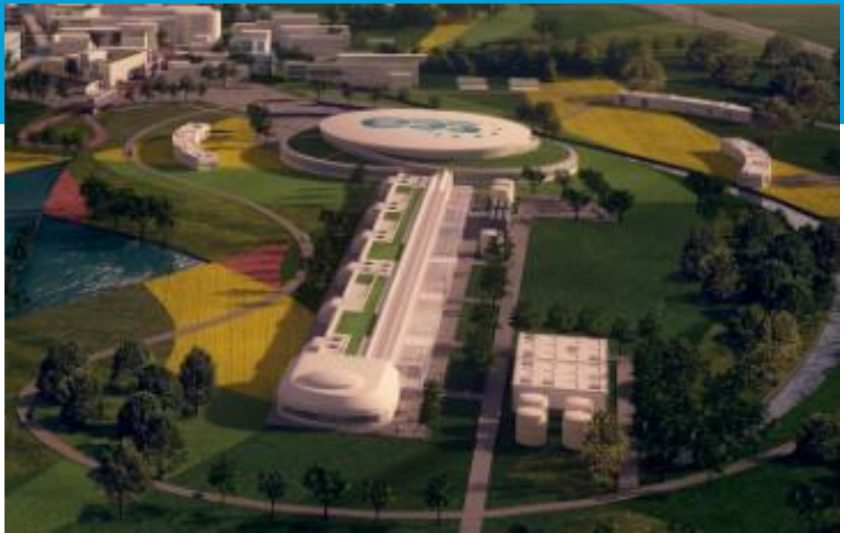


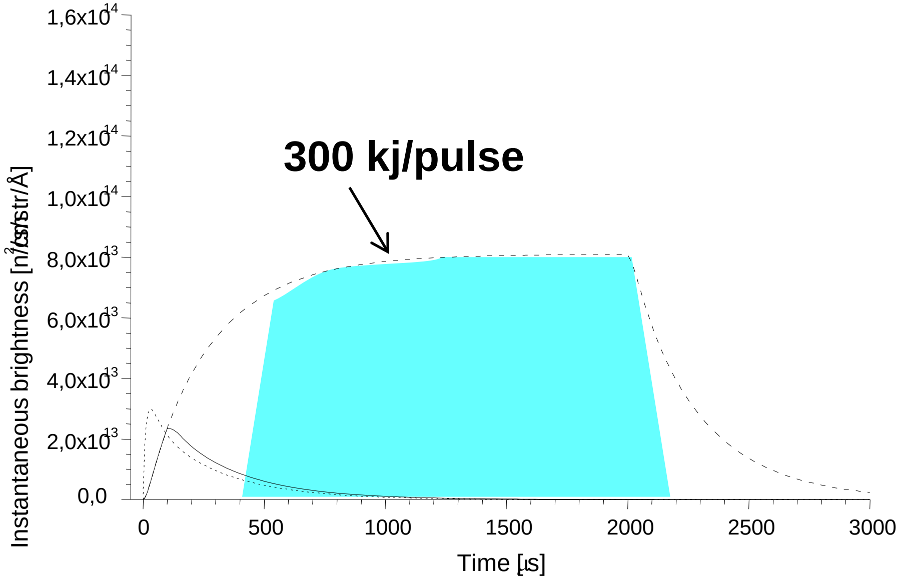


Cost equivalent linear accelerator alone can produce the same cold neutron pulses **by ~100 μs proton pulses at ~ 0.15 GW instantaneous power** → Leave the linac on for **more neutrons per pulse and higher peak brightness…** and use mechanical pulse shaping

→ **Long Pulse source**

# long pulse sources



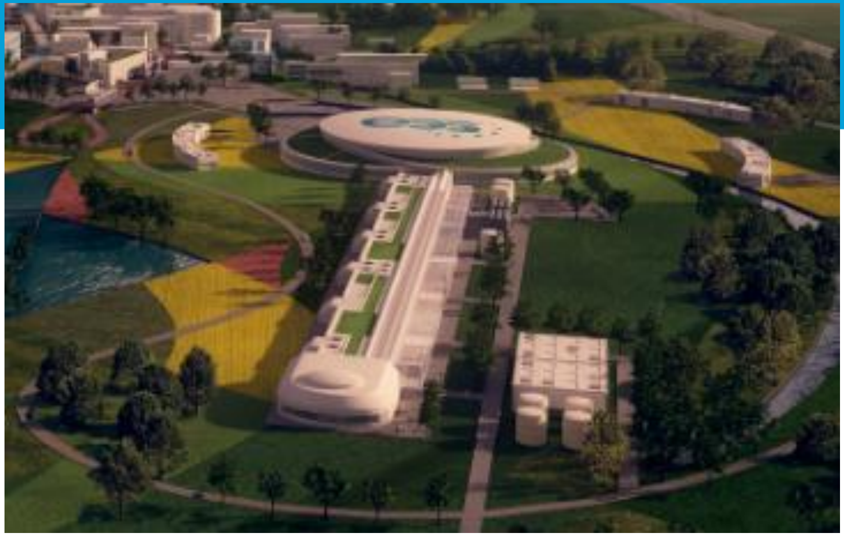


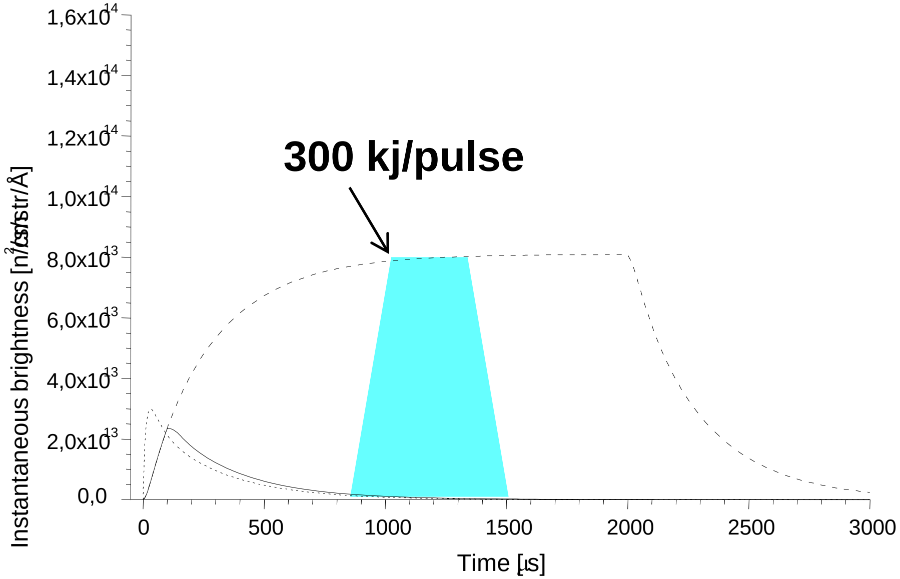
Cost equivalent linear accelerator alone can produce the same cold neutron pulses **by ~100 µs proton pulses at ~ 0.15 GW instantaneous power** → Leave the linac on for **more neutrons per pulse and higher peak brightness…** and use mechanical pulse shaping

→ **Long Pulse source**

**ESS:** 5 MW accelerator power
→ **more neutrons for the same costs and reduced complexity**

# long pulse sources





Cost equivalent linear accelerator alone can produce the same cold neutron pulses **by ~100 μs proton pulses at ~ 0.15 GW instantaneous power** → Leave the linac on for **more neutrons per pulse and higher peak brightness…** and use mechanical pulse shaping → **Long Pulse source**

**ESS:** 5 MW accelerator power → **more neutrons for the same costs and reduced complexity**

(F. Mezei)

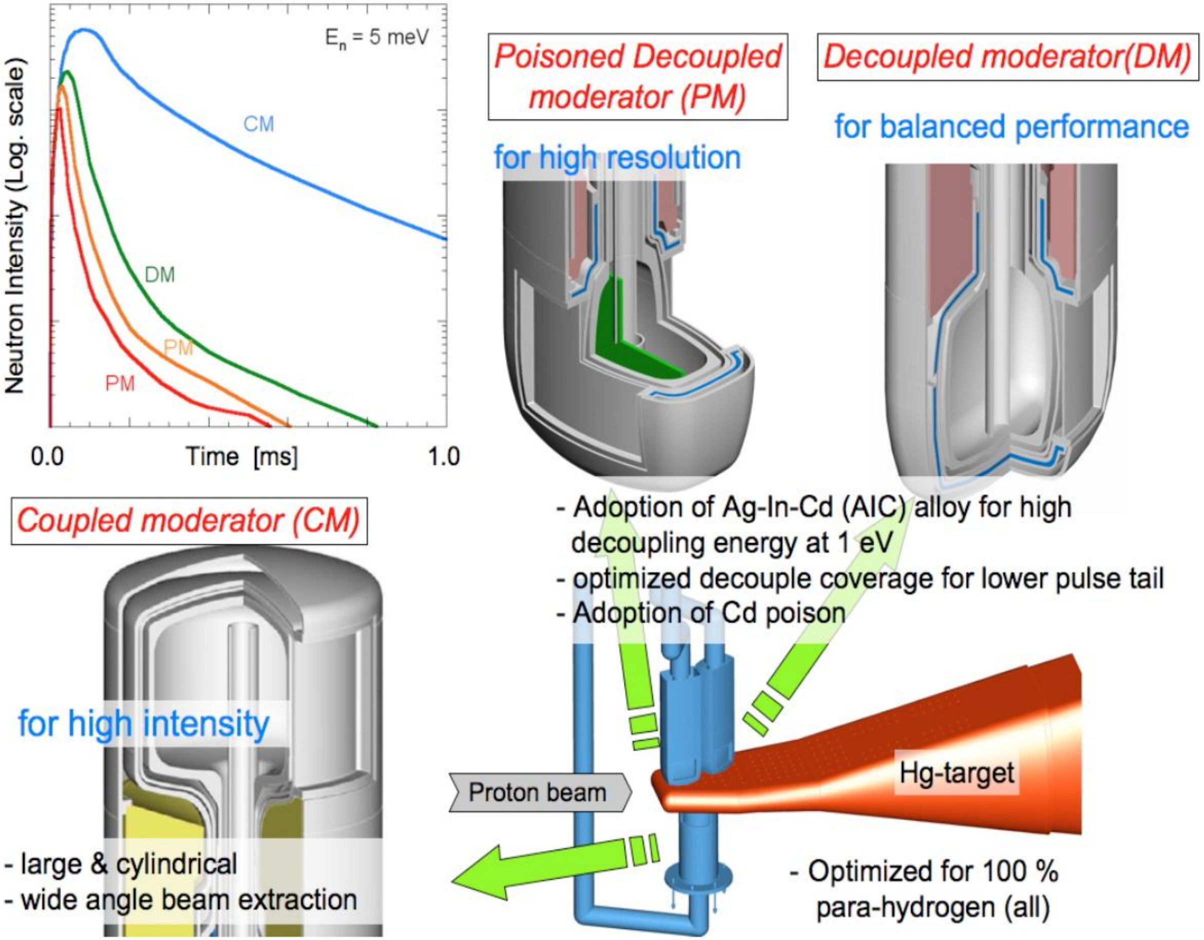
# Moderator decoupling and poisoning

Decoupled moderators are moderators that are wrapped in a layer of a material with a high thermal neutron absorption cross-section on all sides except the viewed surface.
This decoupling layer (e.g. cadmium) prevents thermal neutrons from bouncing back and forth between the moderator and reflector. These neutrons are the main contribution to the long tail of the neutron emission time distribution; thus, absorbing them significantly shortens the neutron pulse length.

Decoupling reduces the brigthness, since it simply absorbs neutrons. However, decoupling signicantly increases the time resolution for experiments, which benefits many experiments.

Another way to increase time resolution, again at the cost of brightness, is to apply a neutron poison to the moderator: mixing an absorbing material into the moderator material. The poison reduces the lifetime of a cold or thermal neutron inside the moderator, resulting in an even shorter tail of the time distribution.

# JPARC: three hydrogen moderators of JSNS: coupled, decoupled, poisoned



*Poisoned Decoupled moderator (PM)*

for high resolution

*Decoupled moderator(DM)*

for balanced performance

- Adoption of Ag-In-Cd (AIC) alloy for high decoupling energy at 1 eV
- optimized decouple coverage for lower pulse tail
- Adoption of Cd poison

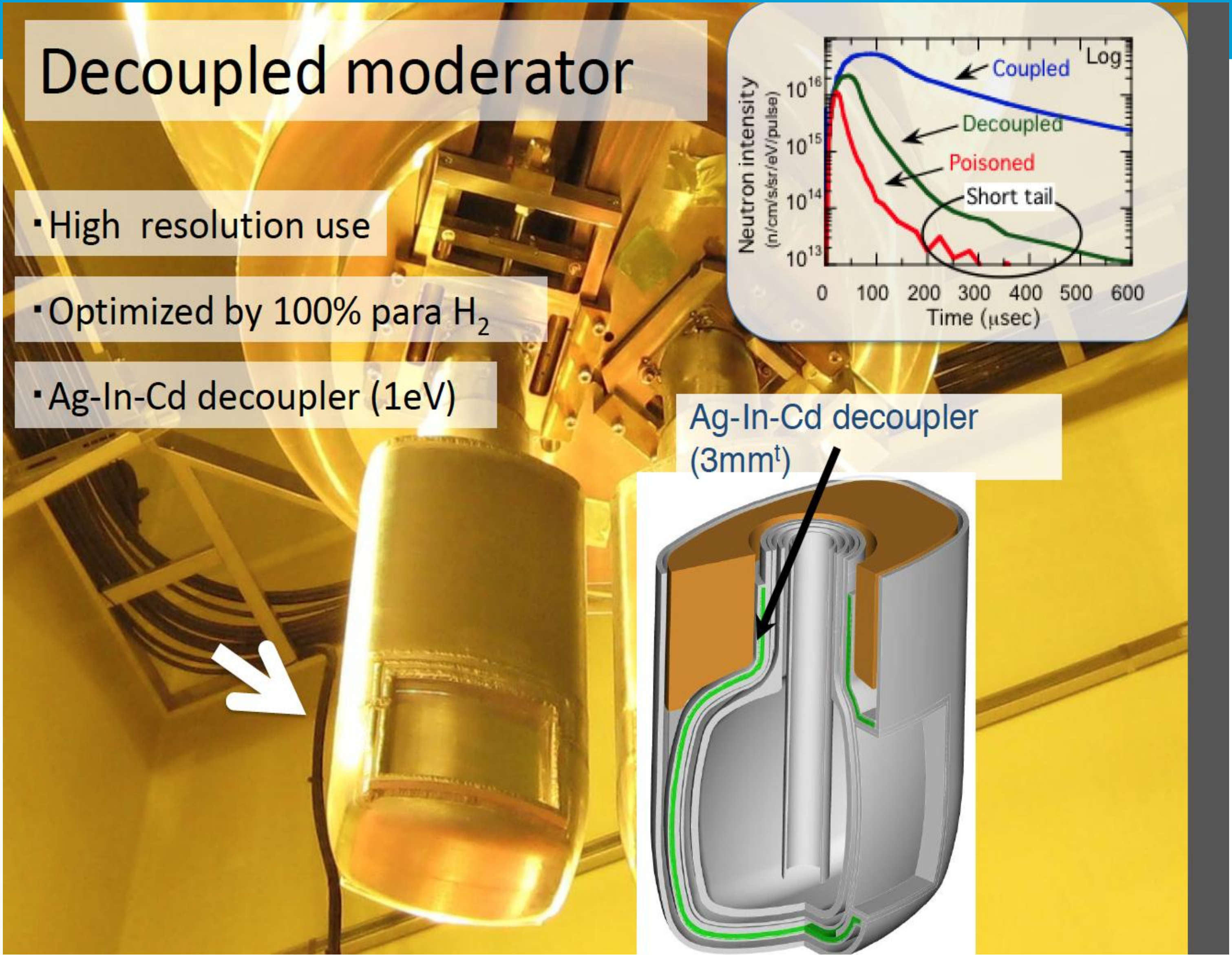
*Coupled moderator (CM)*

for high intensity

- large & cylindrical
- wide angle beam extraction

- Optimized for 100 % para-hydrogen (all)

# JPARC

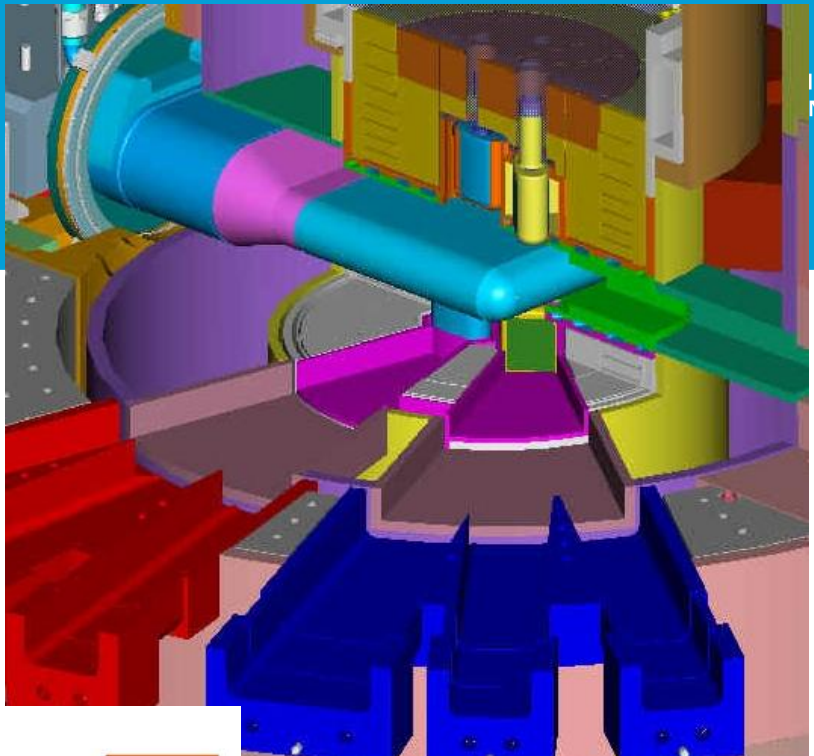


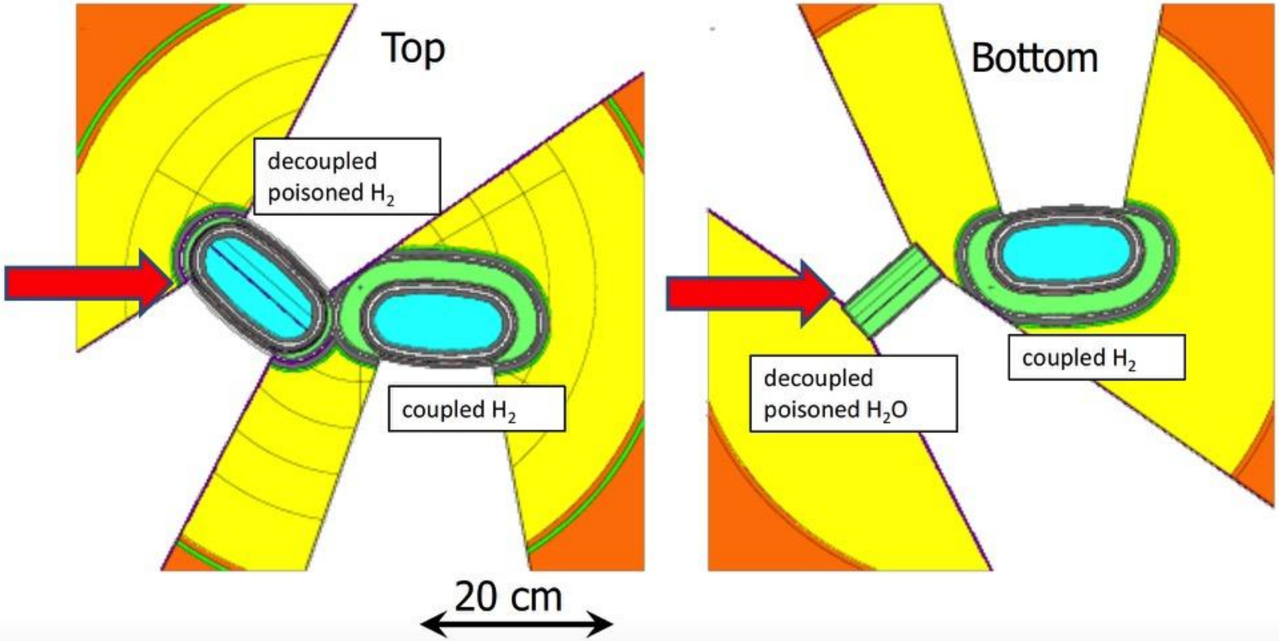
## Decoupled moderator

- High resolution use
- Optimized by 100% para $H_2$
- Ag-In-Cd decoupler (1eV)

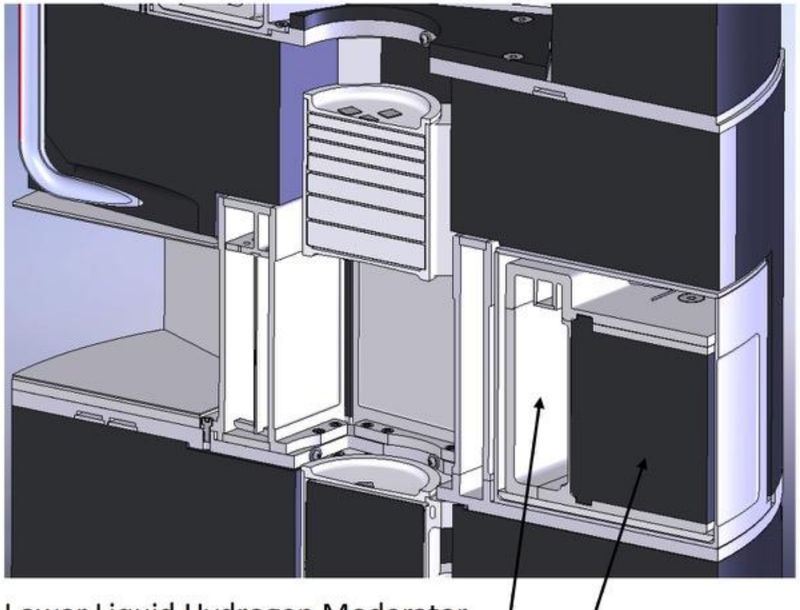
Ag-In-Cd decoupler ($3mm^t$)

# SNS



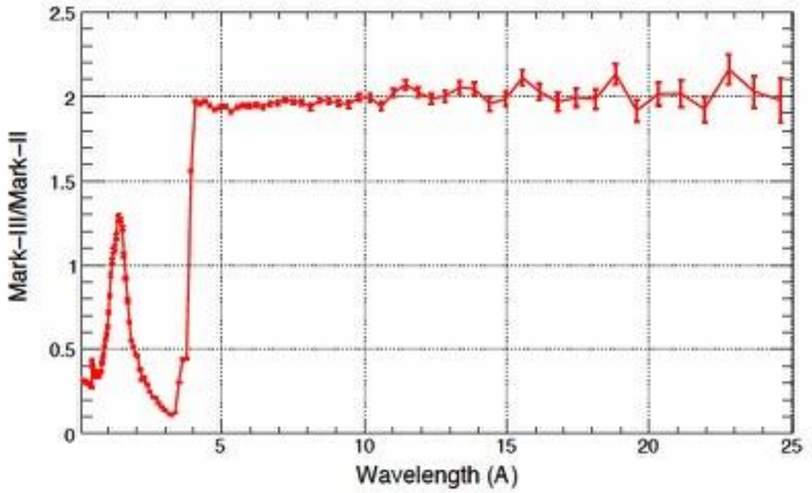

Top
decoupled poisoned $H_2$
coupled $H_2$
Bottom
coupled $H_2$
decoupled poisoned $H_2O$
20 cm

# LANSCE
# flux trap configuration, use of Be filter-reflector



Lower Liquid Hydrogen Moderator

Cold Beryllium Reflector/Filter



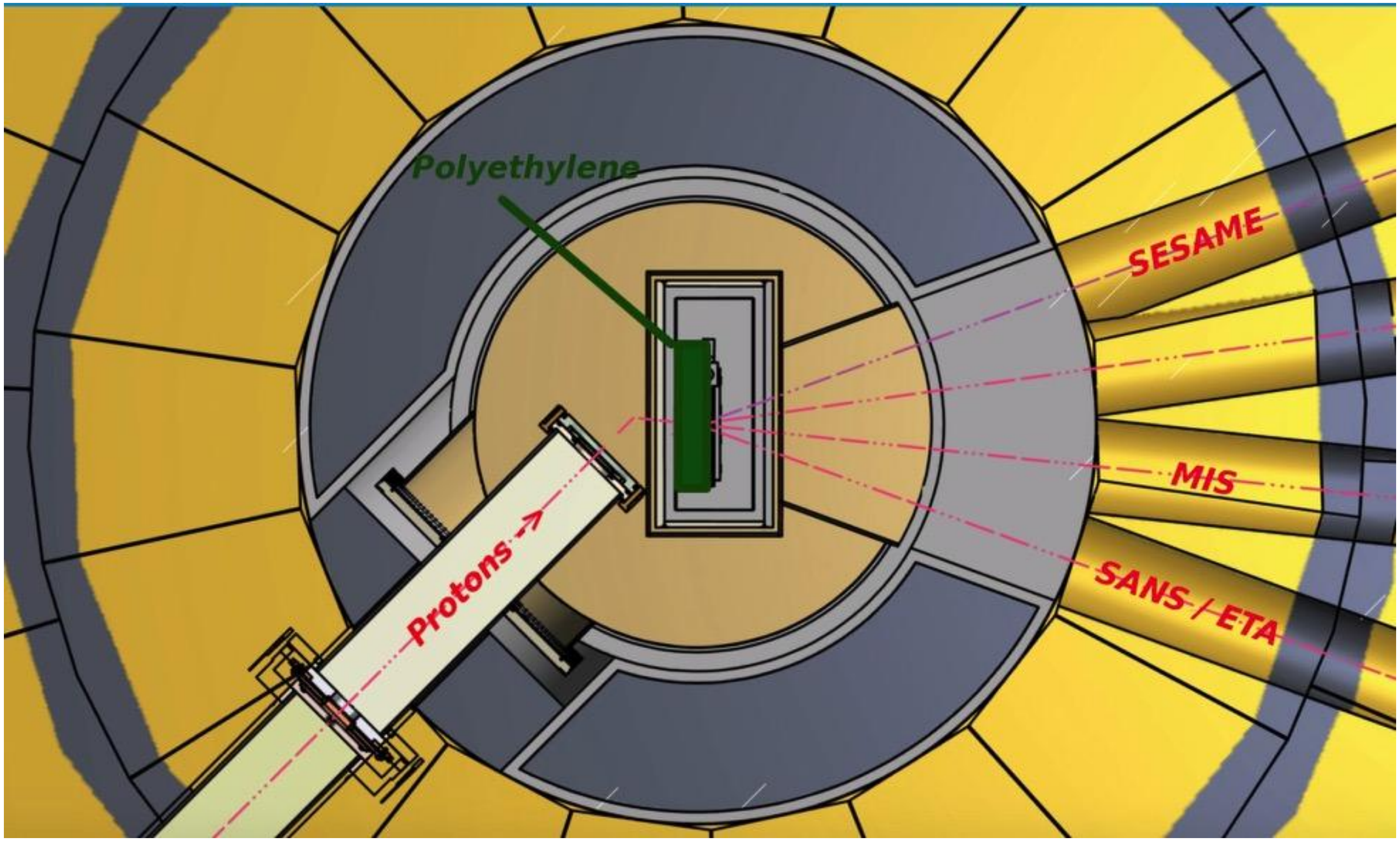
# Less than 1/1000000 of created neutrons reach the sample

- The generation of the prompt neutrons and gammas is driven by the proton beam incident on the liquid mercury target.
- A fraction of the neutrons scatter eventually in the moderators and/or its vicinity towards a beamline and leak into the core vessel insert opening at about one meter distance from the moderator.
- About 33 neutrons per proton are generated in the target station.
- About 0.4 neutrons per proton leak into one of the 18 core vessel openings,
- about 0.001 neutrons per proton have flight directions within one degree of a nominal beam direction and have the potential of exiting the target monolith,
- only 10% of those are in the thermal energy range and therefore of potential use for scattering instruments.
- *Nature is not in favor of neutron scattering.*

(Estimate of F. Gallmeier for SNS)

# Compact sources are suitable for moderator optimization

LENS (Indiana University)



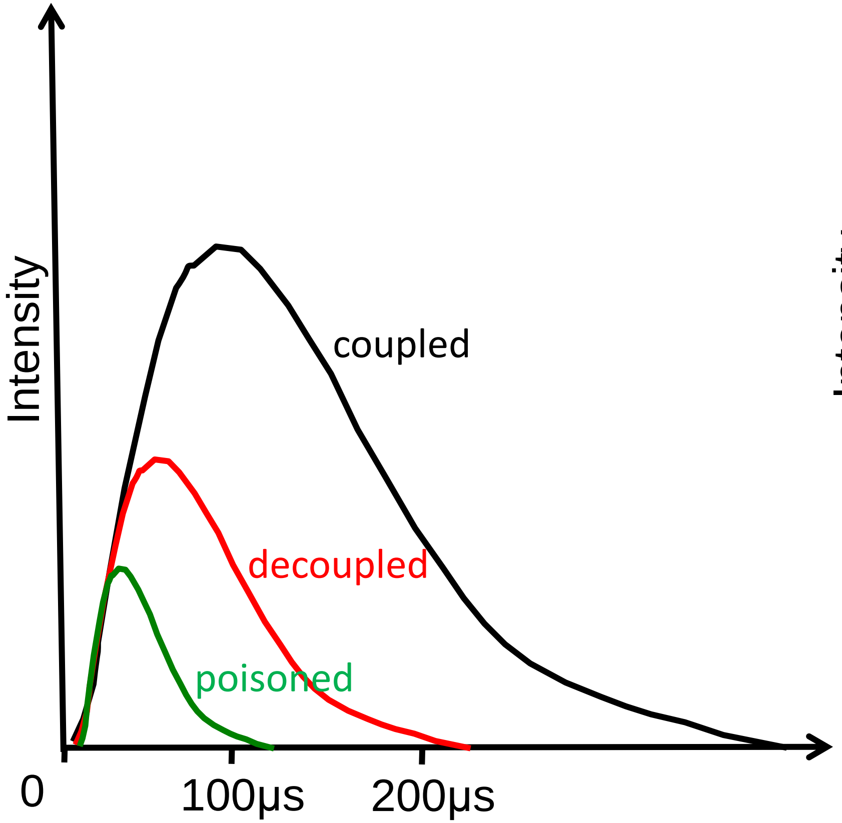
# Long pulse vs short pulse: difference on moderators

- In short pulse sources, a pulse width of slow-neutrons is determined by the neutron thermalization and pulse-decay-time in a moderator. Different types of moderators are used in short pulses, depending if intensity or time resolution have priority since the time structure of the pulse is determined by the moderator type.
- In a long pulse, the time structure is determined by the proton pulse. Pulse shaping is determined by choppers outside the target monolith. Therefore, a long pulse facility can accommodate one type of moderator for all beamports.

# Adapting the pulse width

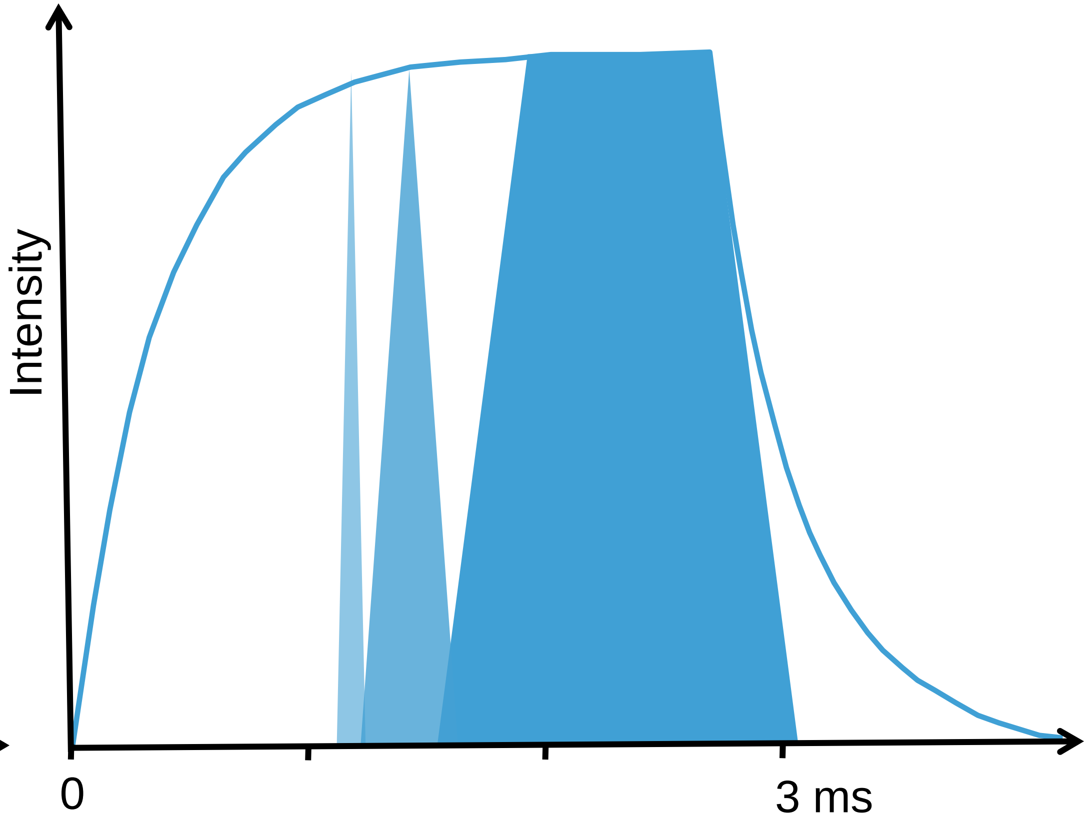
## Short-Pulse Source

- set pulse width by choosing moderator



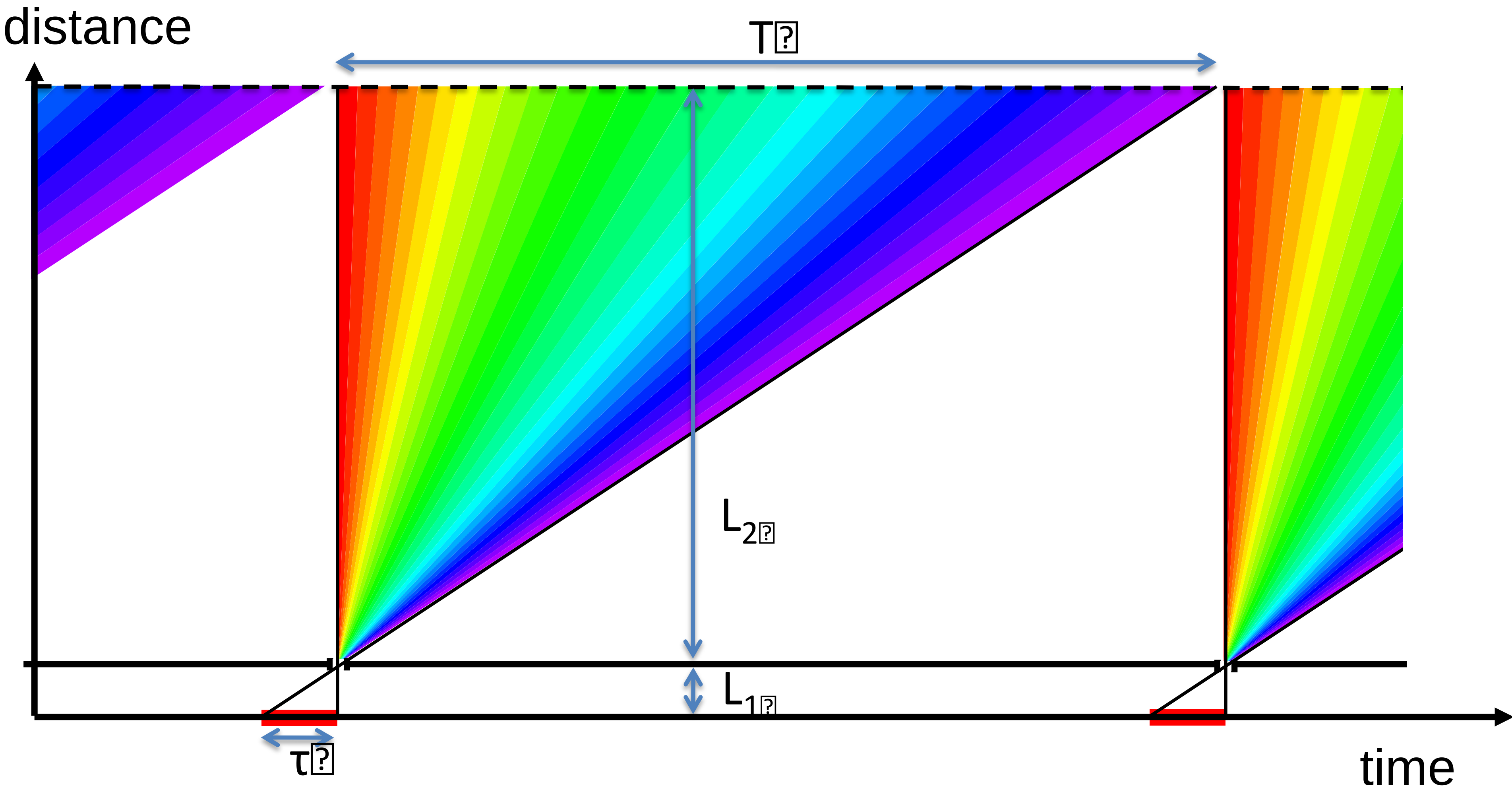
## ESS

- set pulse width using pulse-shaping chopper



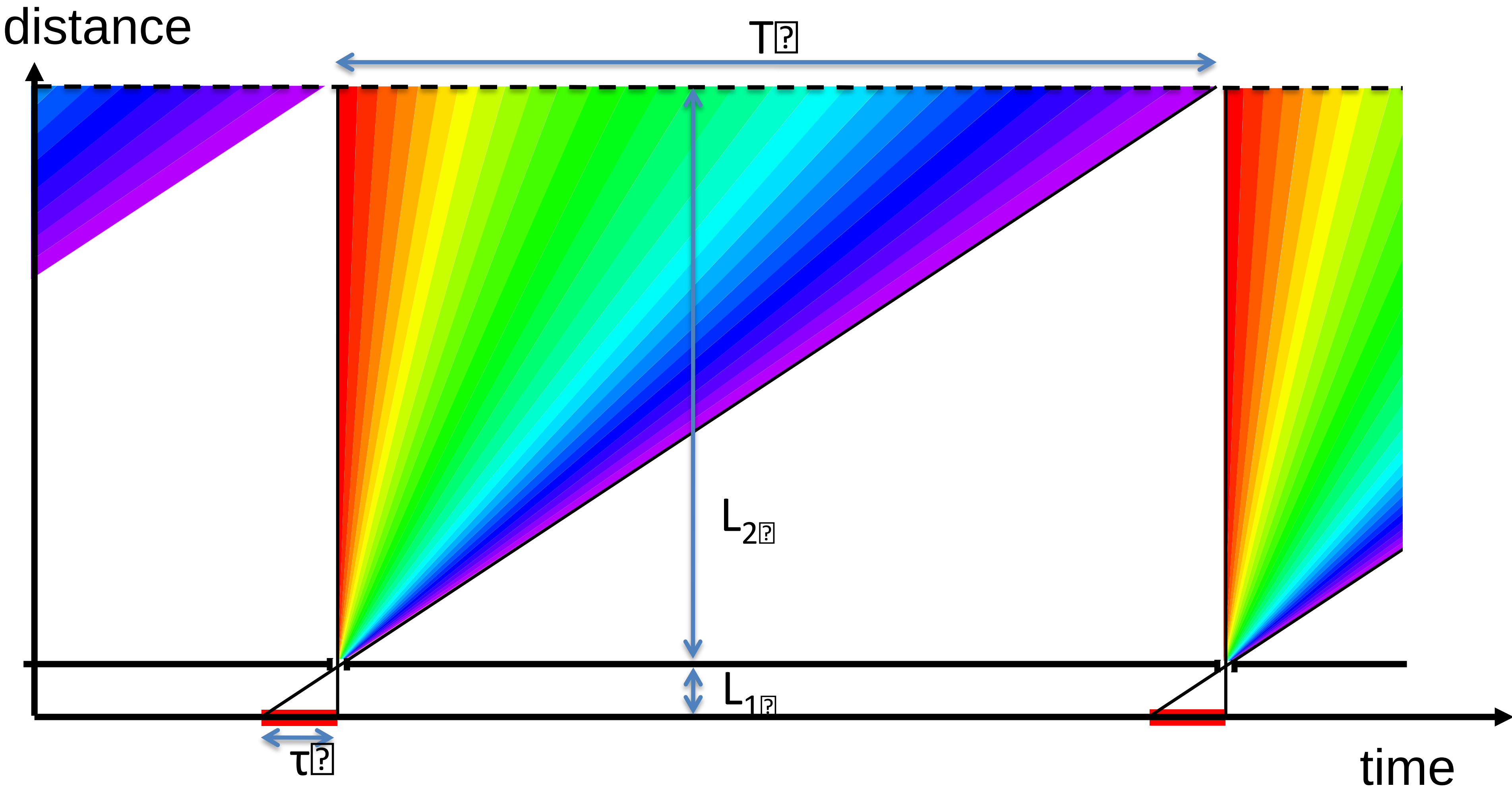
# Impact on bandwidth of pulse-shaping chopper

(K. Andersen)



# Impact on bandwidth of pulse-shaping chopper

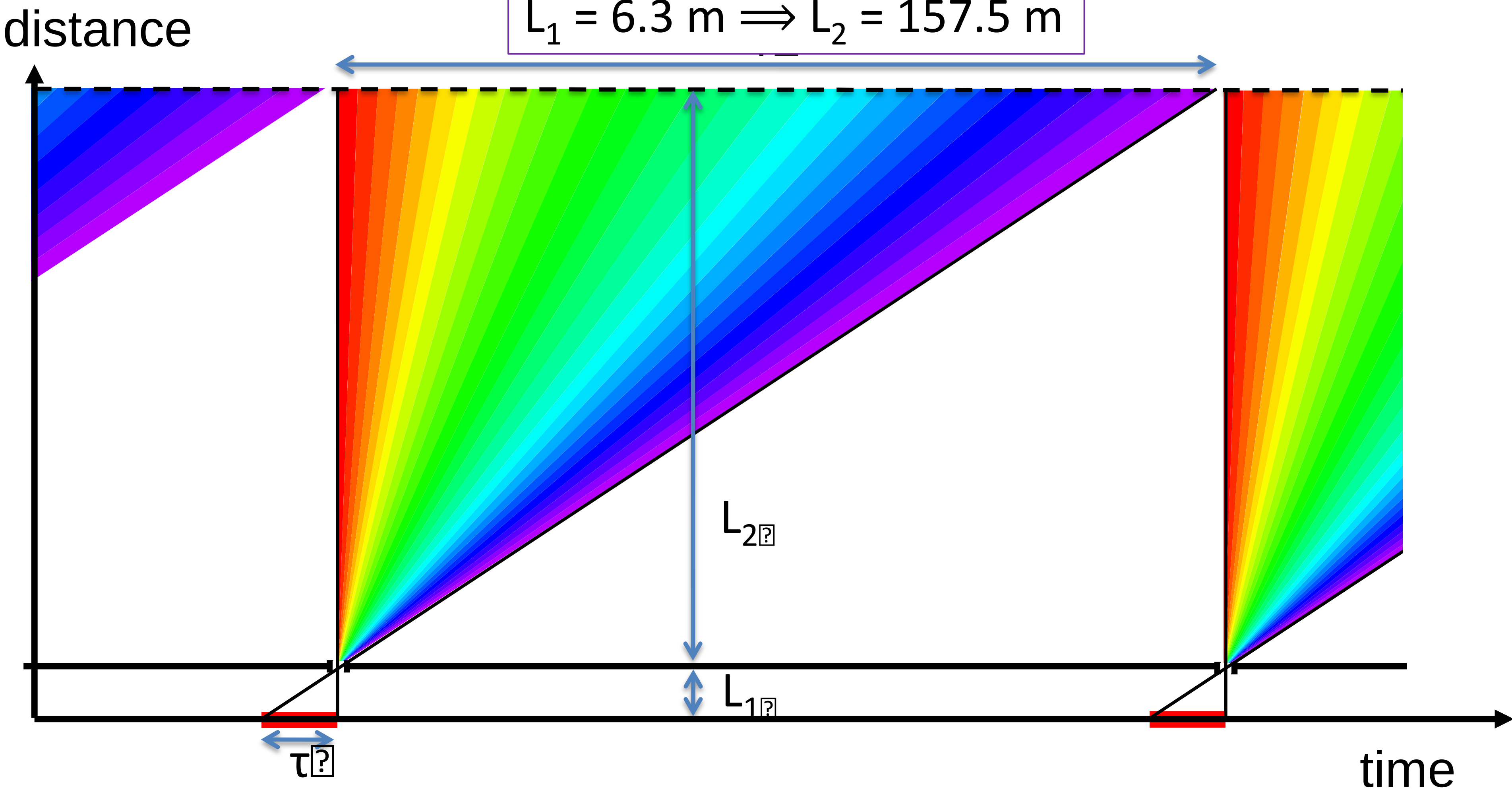
$$T/\tau = 25 \Longrightarrow L_2/L_1 = 25$$



# Impact on bandwidth of pulse-shaping chopper

$T/\tau = 25 \Longrightarrow L_2/L_1 = 25$

$L_1 = 6.3\ \text{m} \Longrightarrow L_2 = 157.5\ \text{m}$

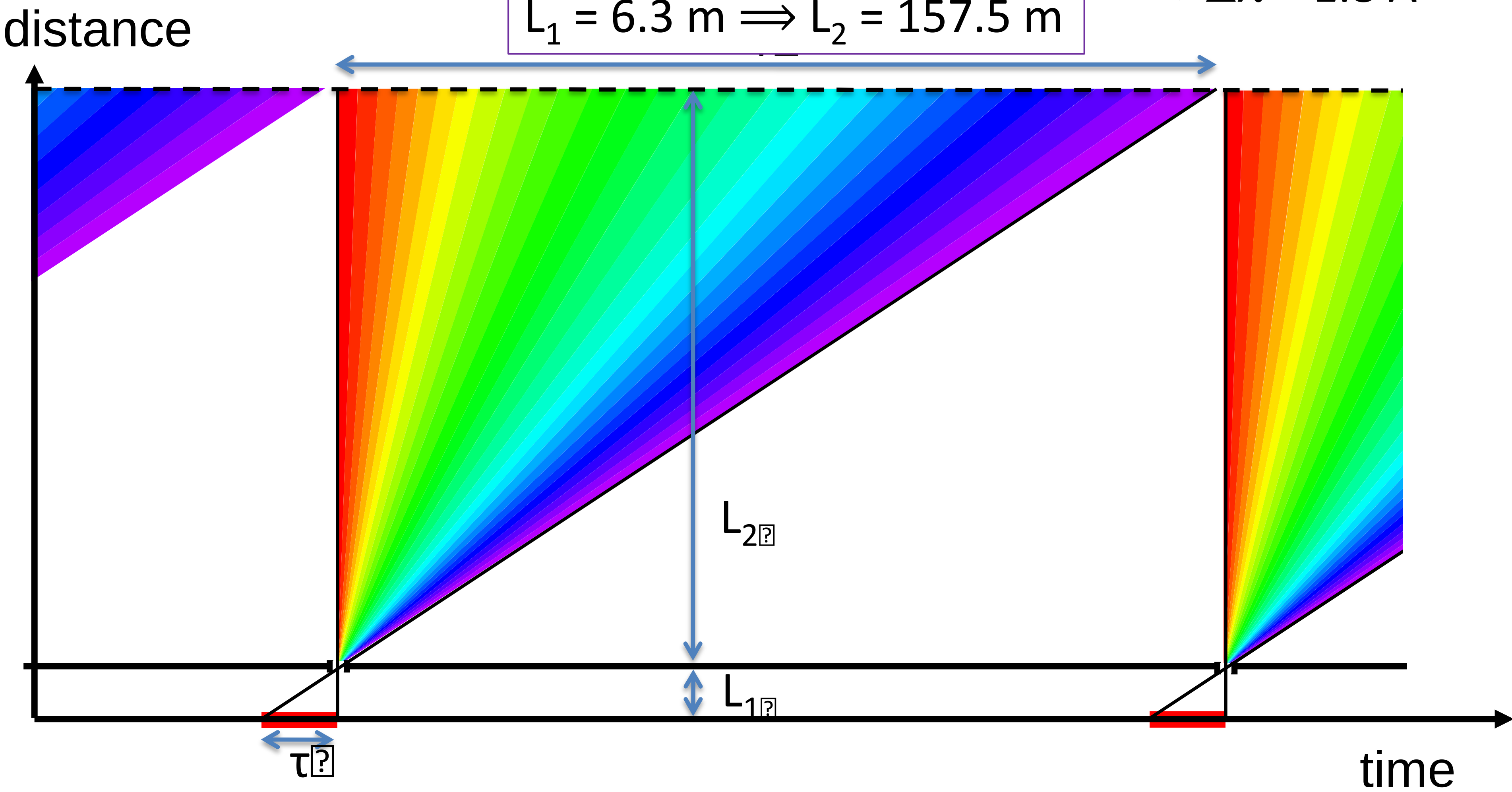


# Impact on bandwidth of pulse-shaping chopper

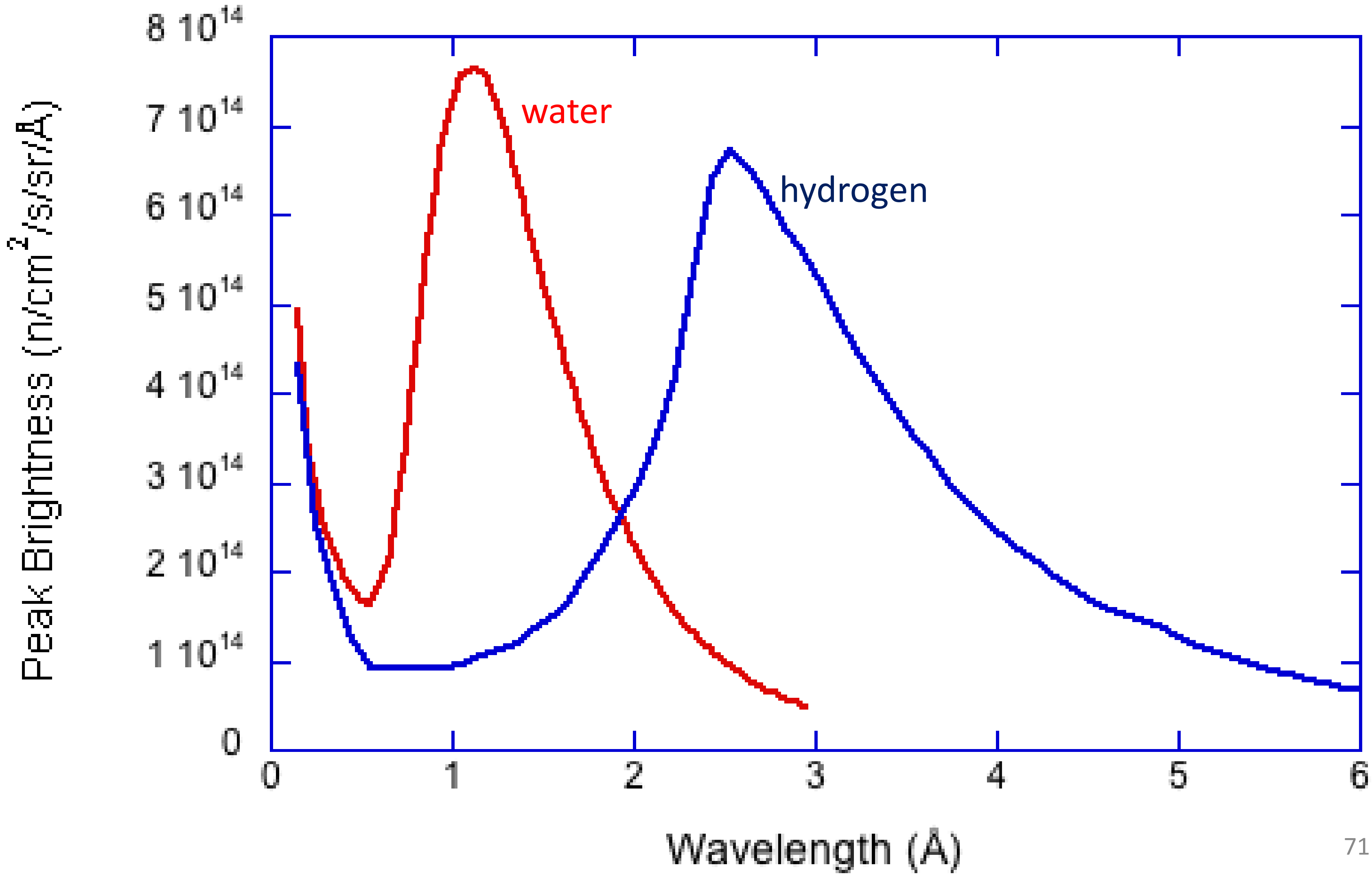
$T/\tau = 25 \Longrightarrow L_2/L_1 = 25$

$L_1 = 6.3\text{ m} \Longrightarrow L_2 = 157.5\text{ m}$

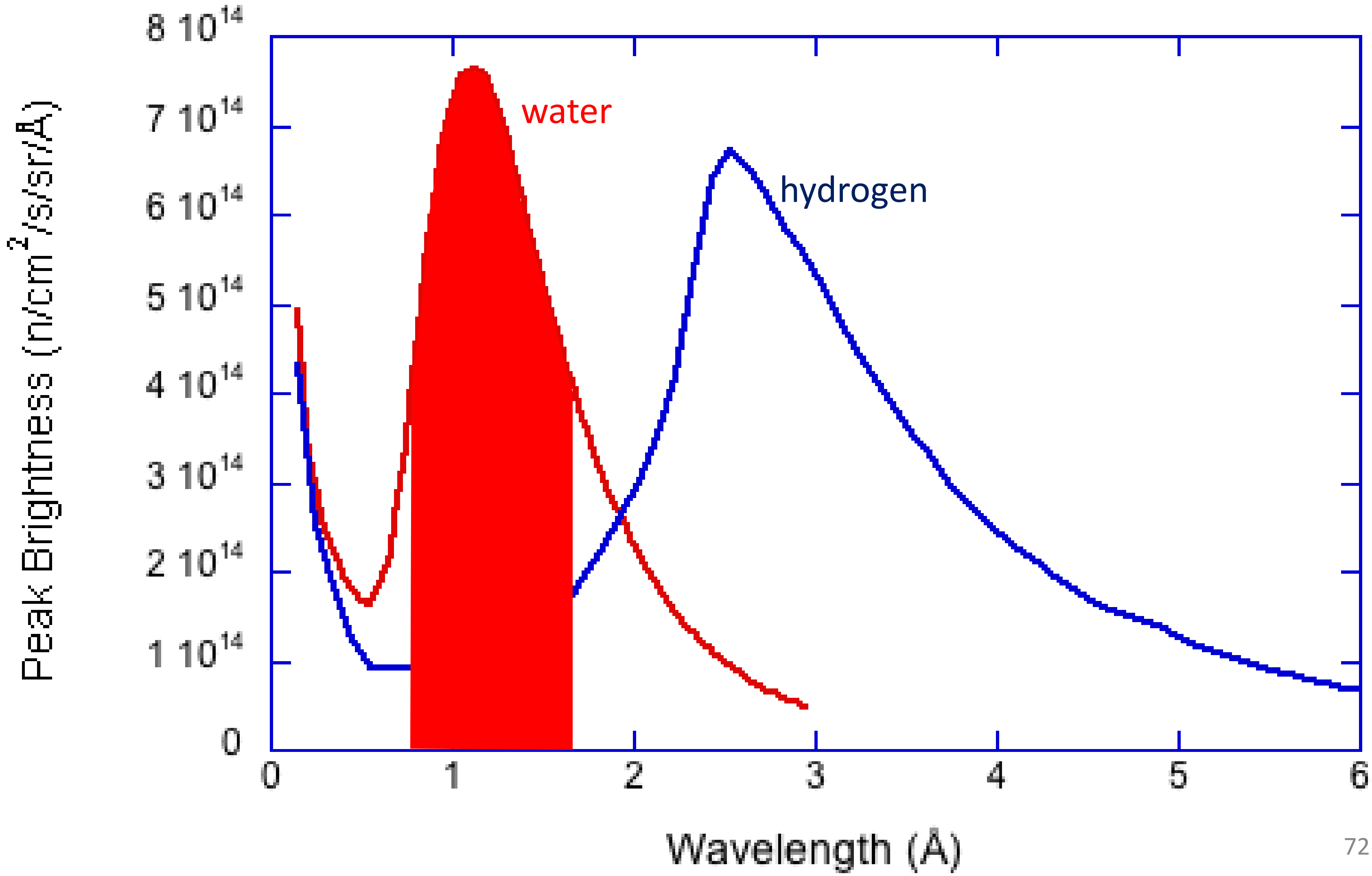
$\Longrightarrow \Delta\lambda = 1.8\text{ Å}$



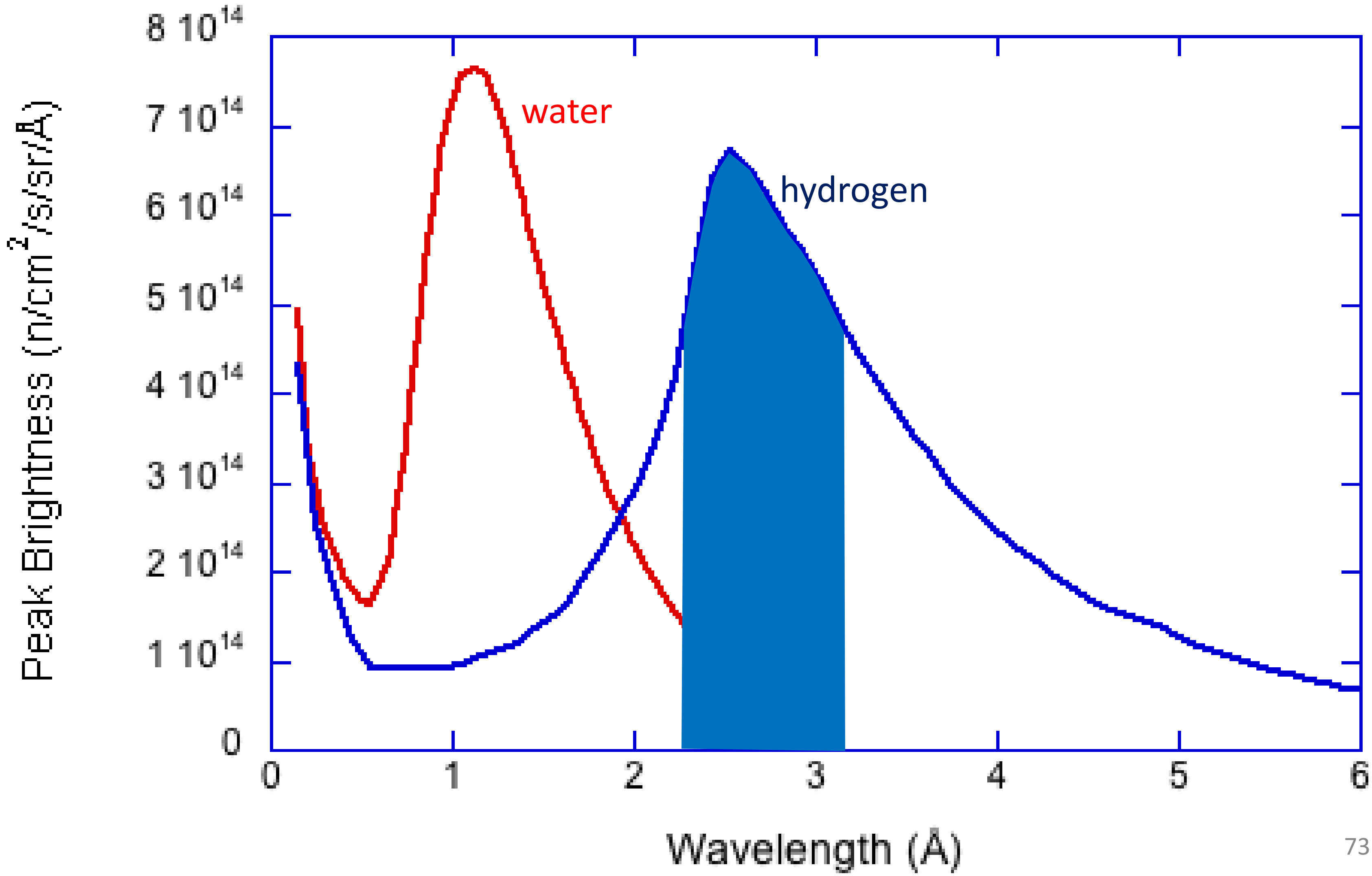
# Impact on bandwidth of pulse-shaping chopper



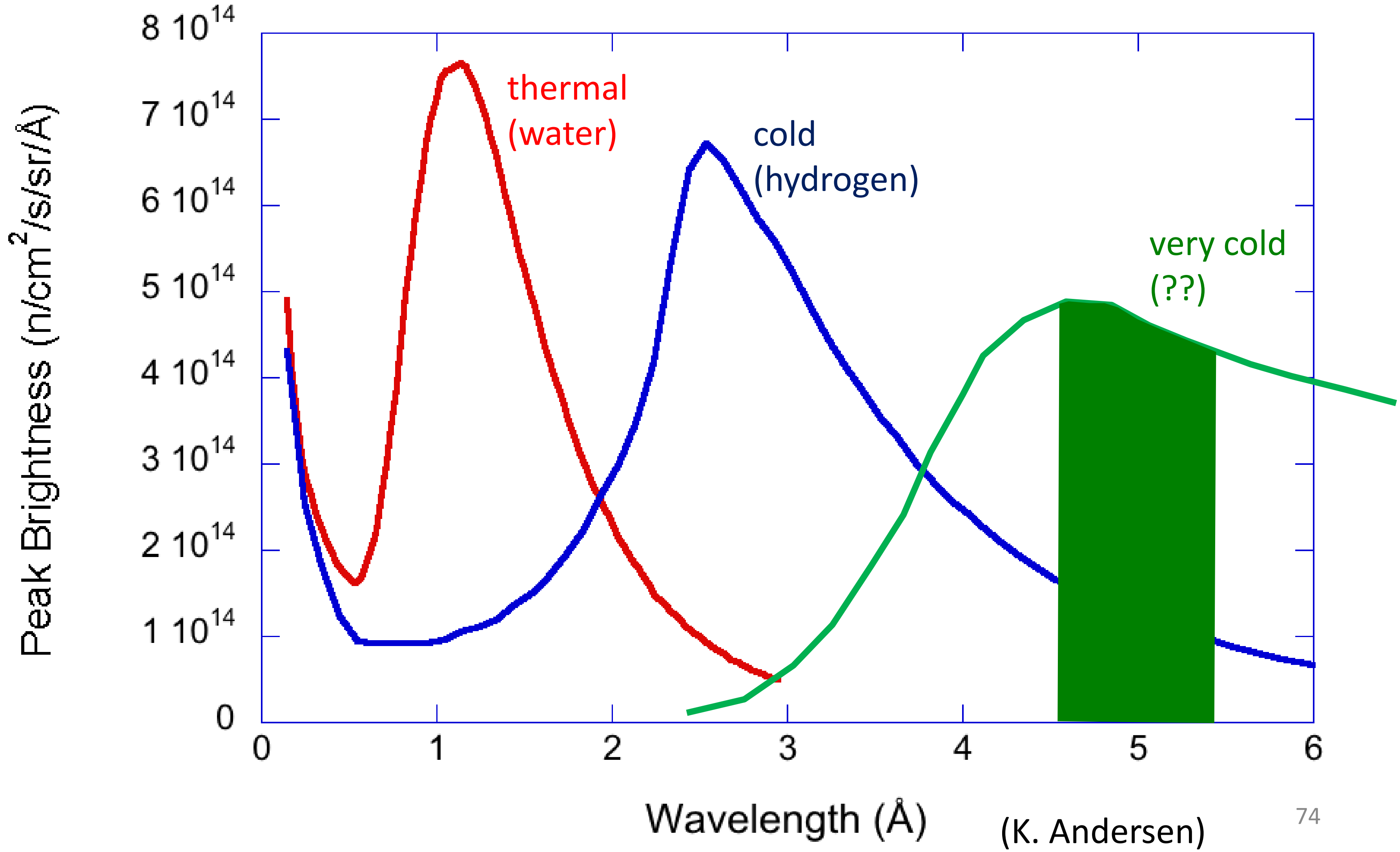
# Impact on bandwidth of pulse-shaping chopper



# Impact on bandwidth of pulse-shaping chopper



# Case for VCN source

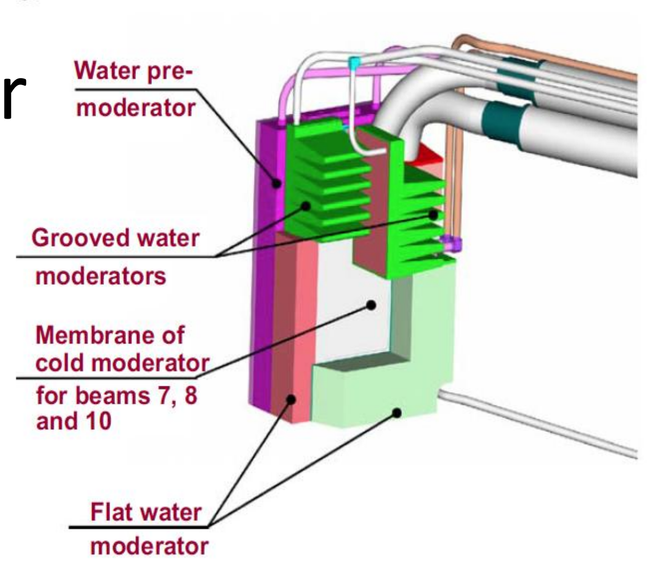


(K. Andersen)

# DIRECTIONAL moderators

- Dream: emit the neutrons in the preferential direction: towards the instruments
- But, neutrons are coming from all directions to the moderator (from the target and from the reflector)
- Can we make neutron scatter in the preferential direction, using specific materials or geometries?

# IBR2 grooved water moderator



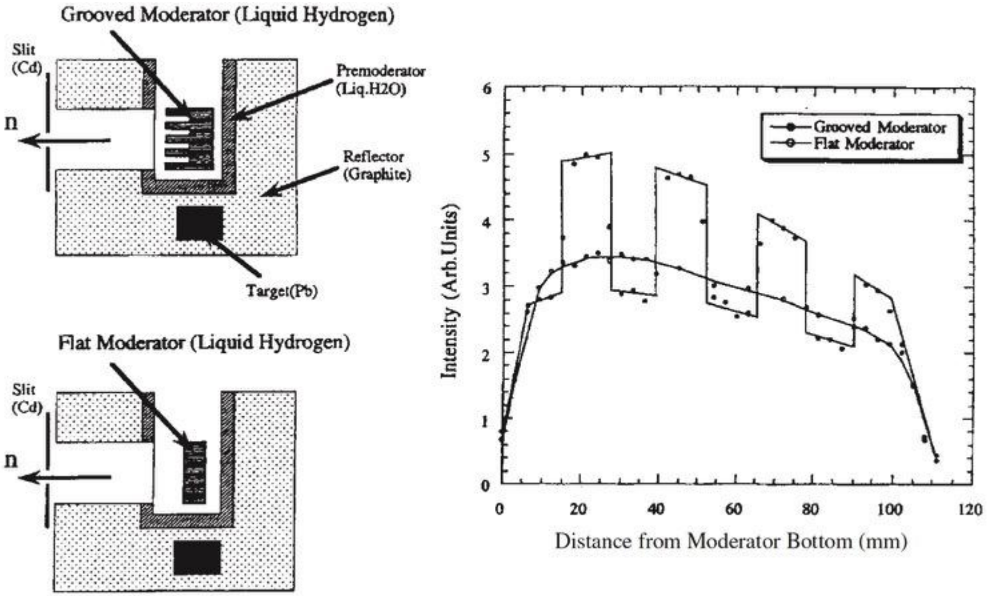
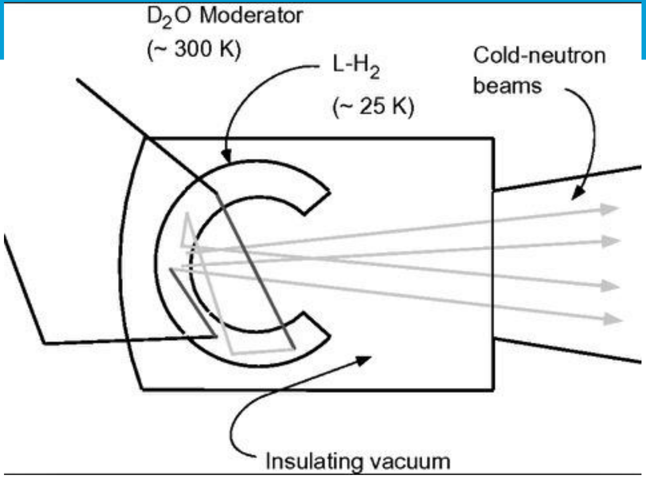
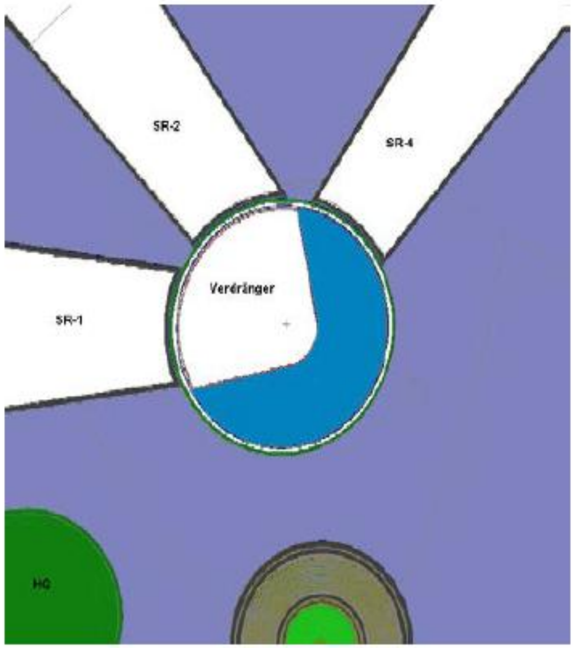


**Figure 29.** Measured spatial distribution of 5 meV neutrons from a grooved $H_2$ moderator with a PM at 20 K (right) with its illustration (left).

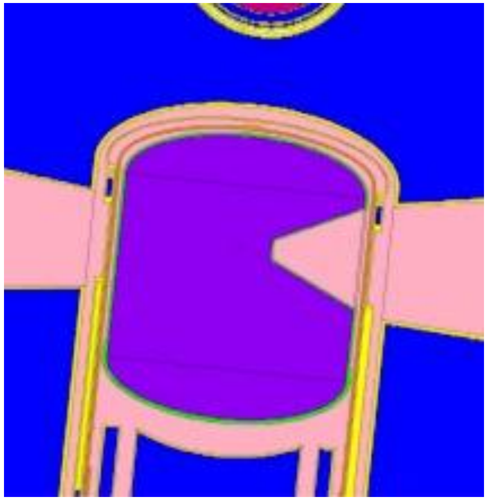
# Reentrant holes



FRM II



SINQ



# The design process of the ESS moderators

- The design of the ESS moderator is a good example of the overall process of optimizing the moderators to provide the highest brightness to the instrument suite.
- It was an iterative process involving an optimization of the full chain from spallation neutron production to slow neutrons at the samples
  - Iterative work of moderator brightness optimization, and optimization of brightness transfer to the instruments for the reference instrument suite
- It had a profound impact on the configuration of the ESS facility

# 16 instruments but available grid of 42 beam ports, bispectral extraction required

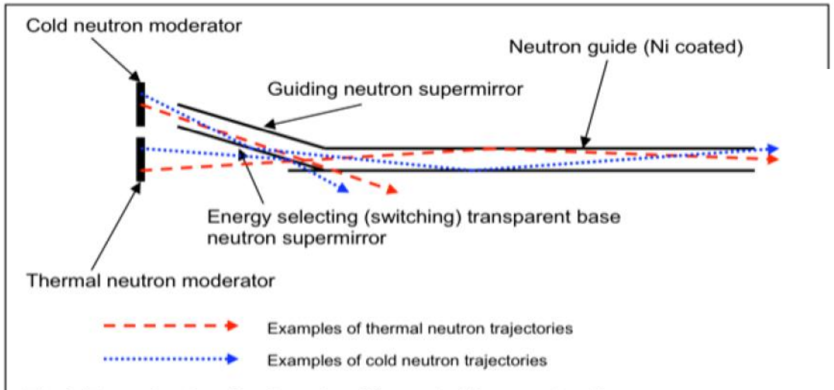
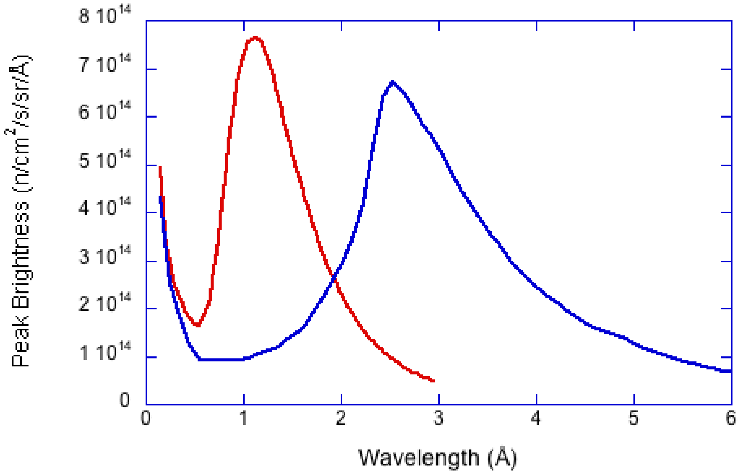
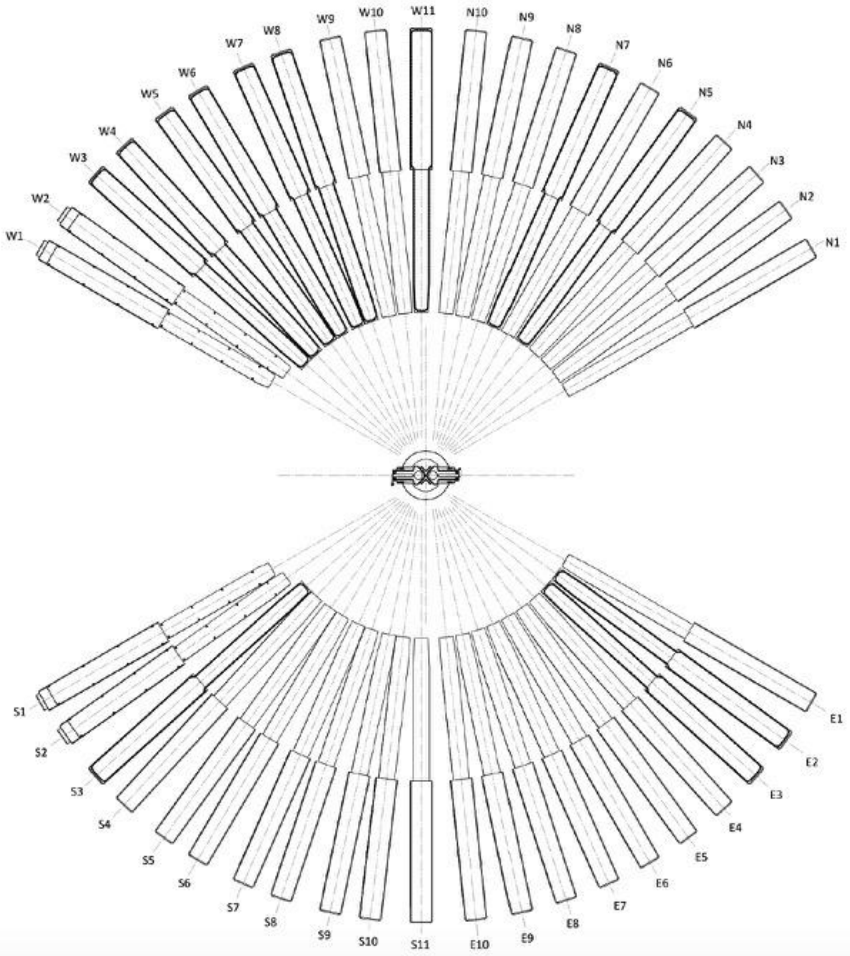


**Fig.1. Example of realization of multi-spectral beam extraction**

(F. Mezei, M. Russina, Patent Berlin, 2002)

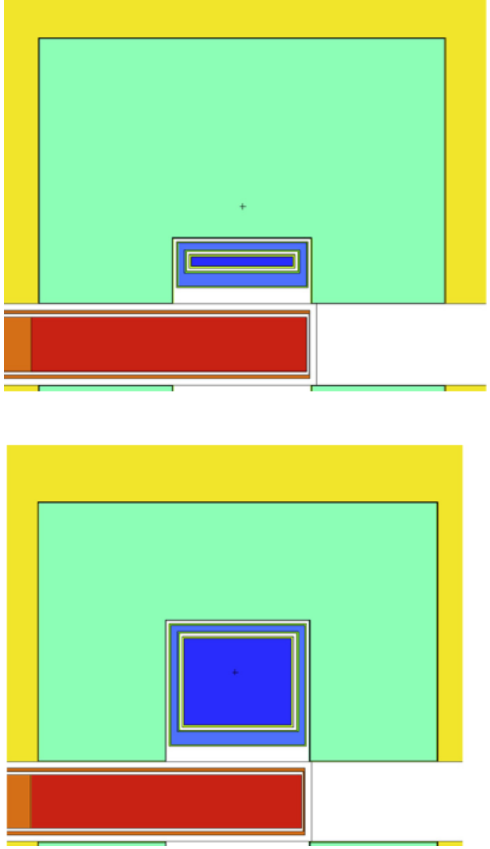


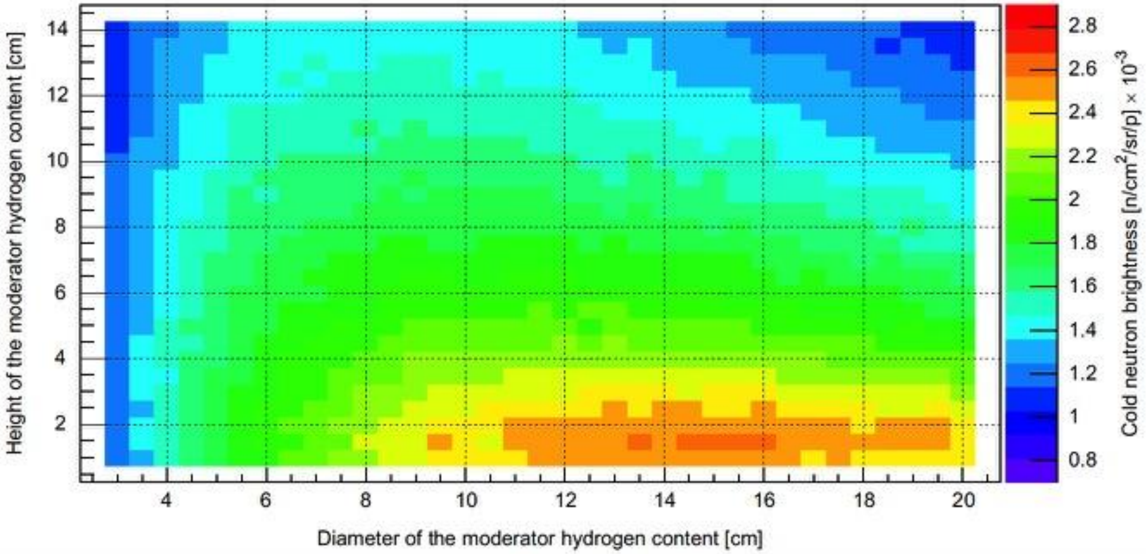


# Brightness optimization

Nuclear Instruments and Methods in Physics Research A 729 (2013) 500–505

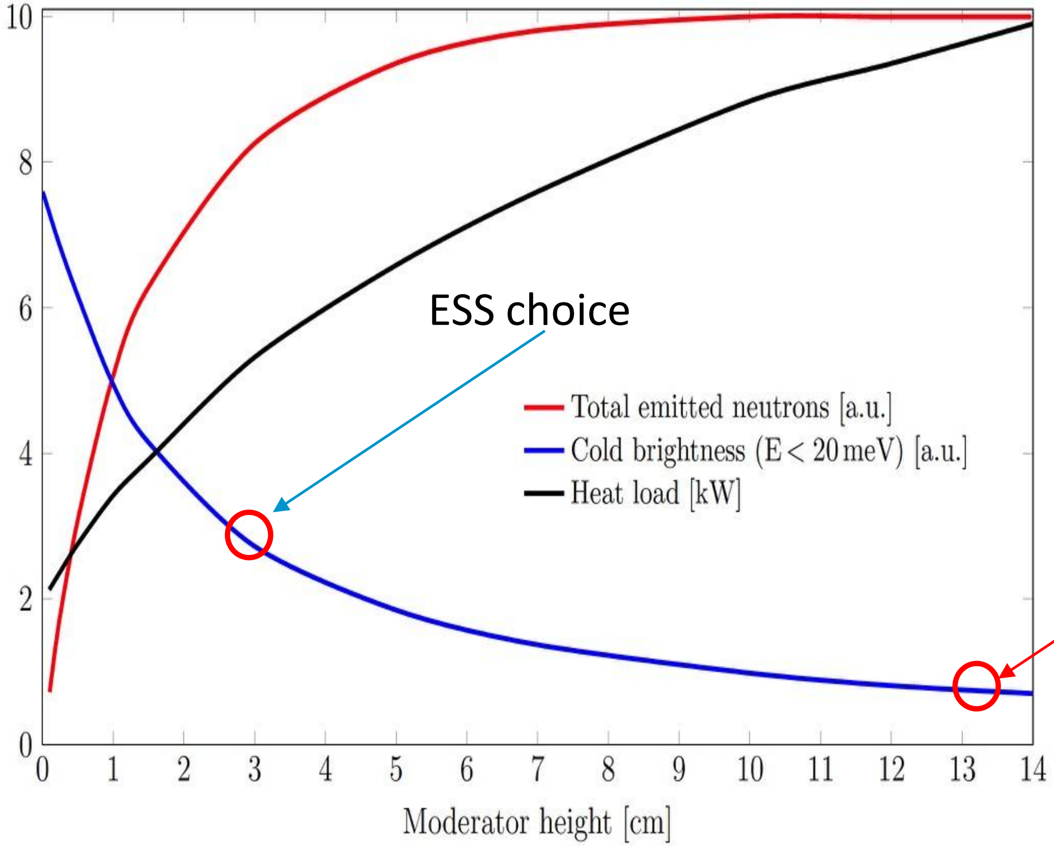
Map of unperturbed brightness



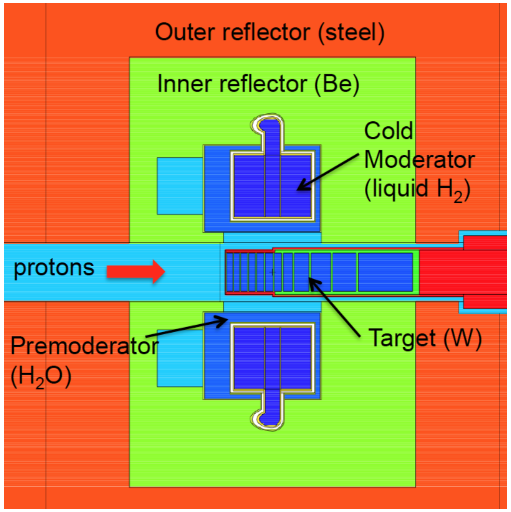


# Less neutrons emitted, but more arrive at the sample

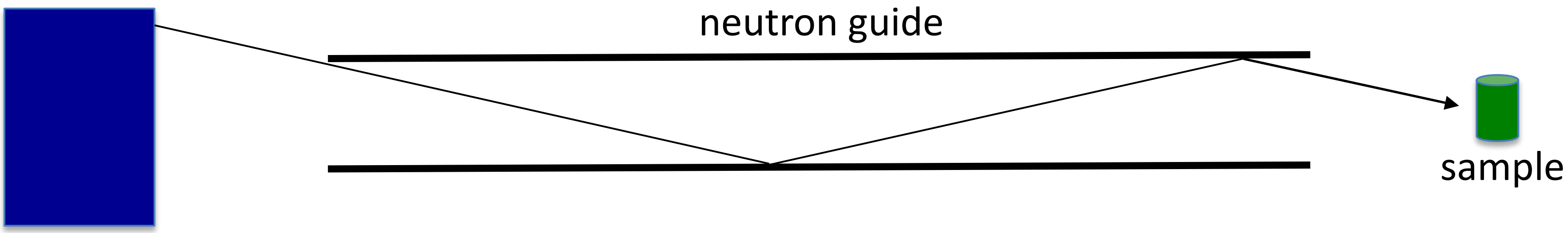
Highest brightness for low moderator thickness must however be confirmed by calculations to the sample



Original ESS design
(Technical Design Report, 2014)



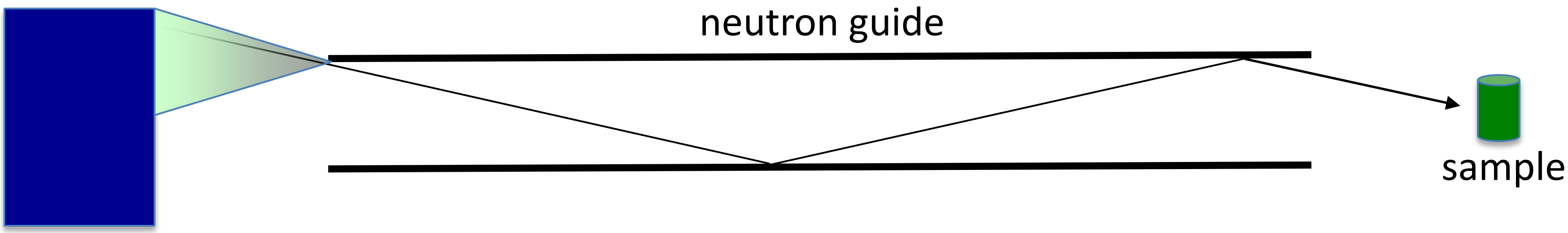
# Guide Illumination



Beam requirements:

- Area
- Divergence
- Wavelength

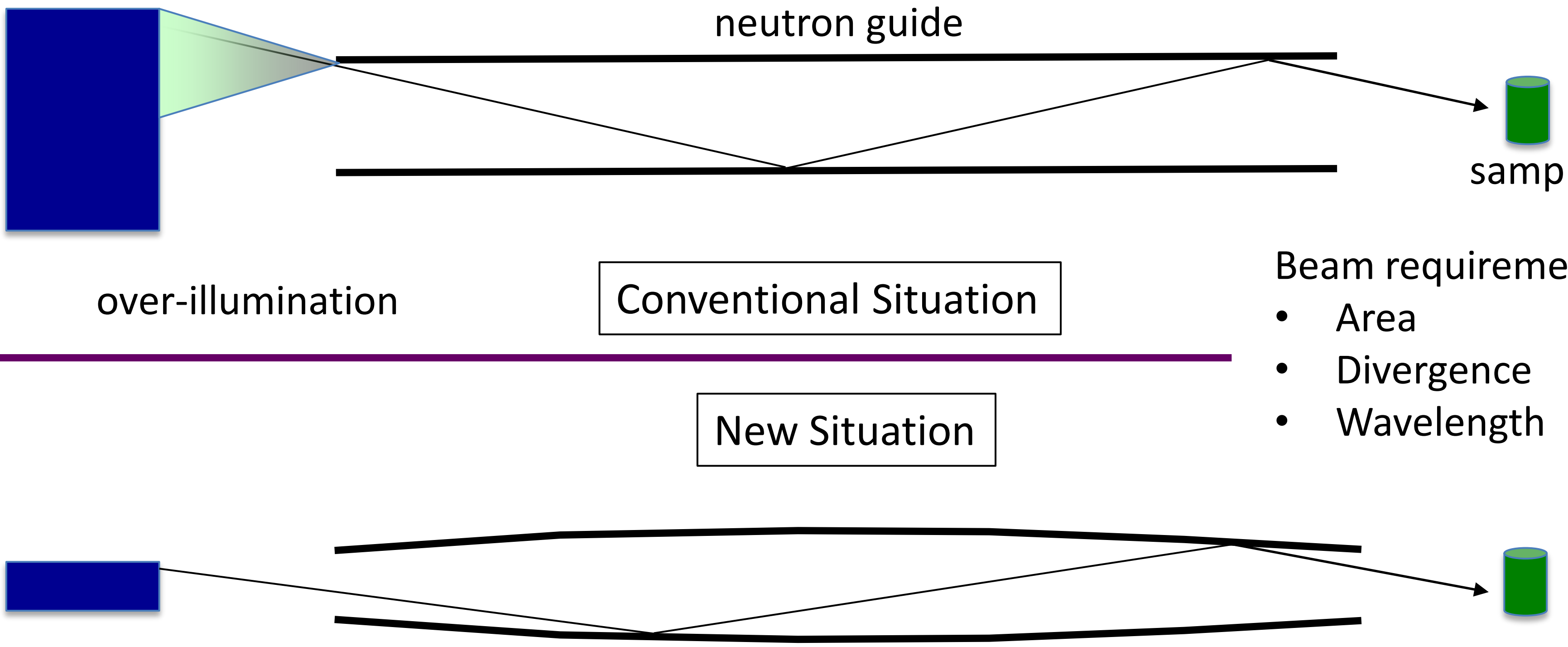
# Guide Illumination



over-illumination

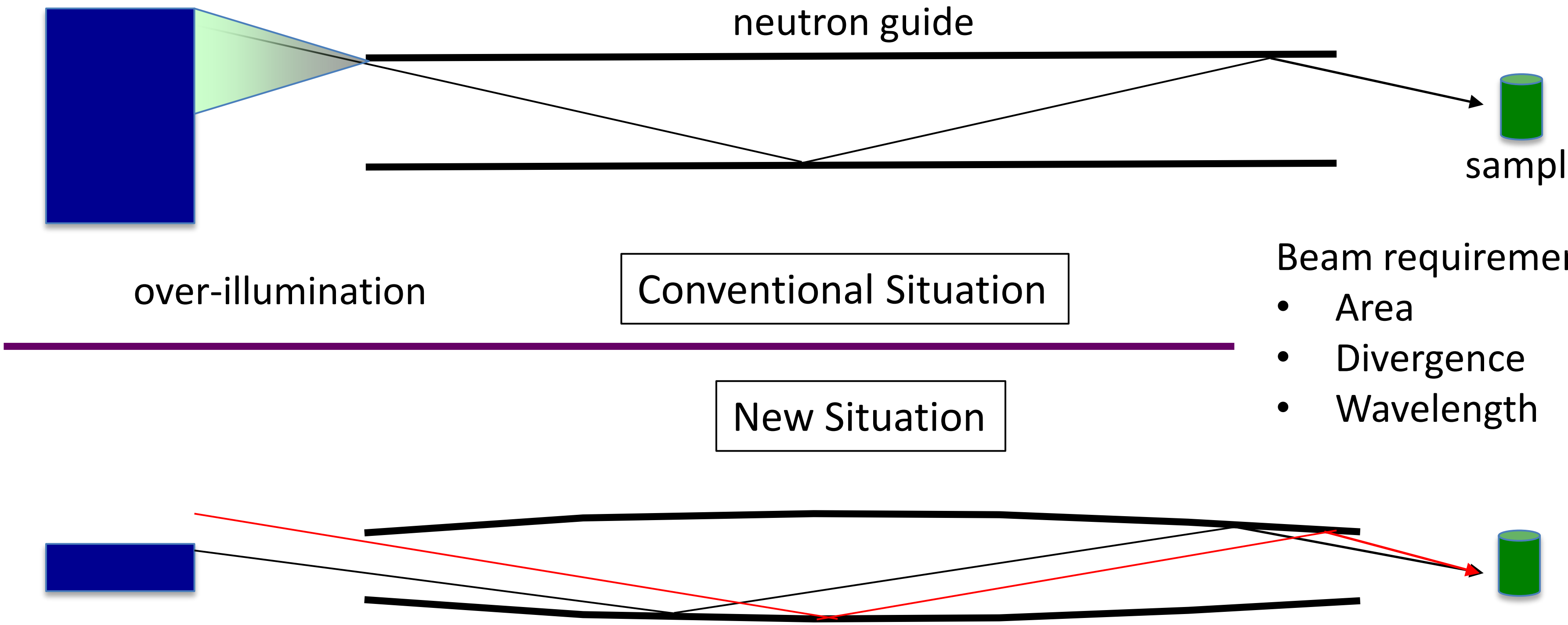
Beam requirements:
- Area
- Divergence
- Wavelength

# Guide Illumination



Beam requirements:
- Area
- Divergence
- Wavelength

# Guide Illumination



neutron guide

sample

over-illumination

Conventional Situation

New Situation

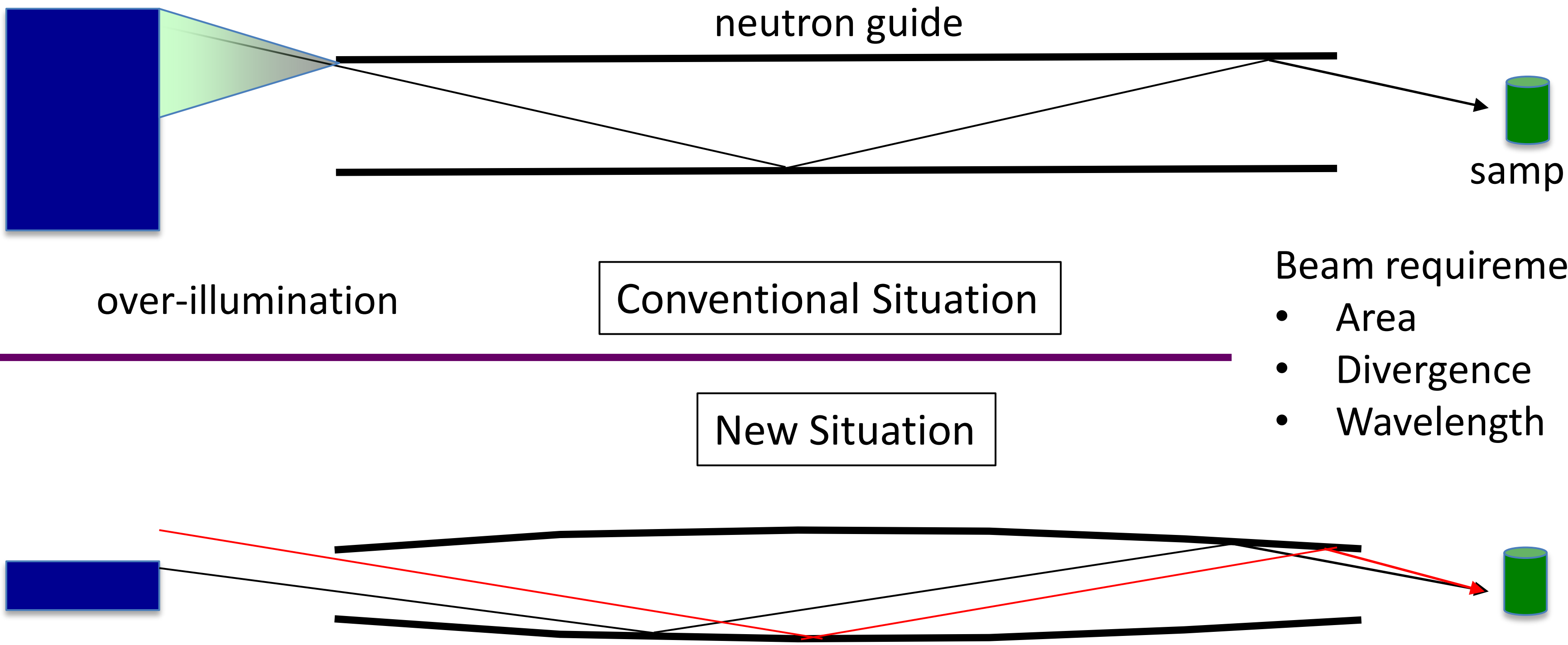
under-illumination

Beam requirements:

- Area
- Divergence
- Wavelength

=> less efficient brilliance transfer

# Guide Illumination



neutron guide

sample

over-illumination

Conventional Situation

New Situation

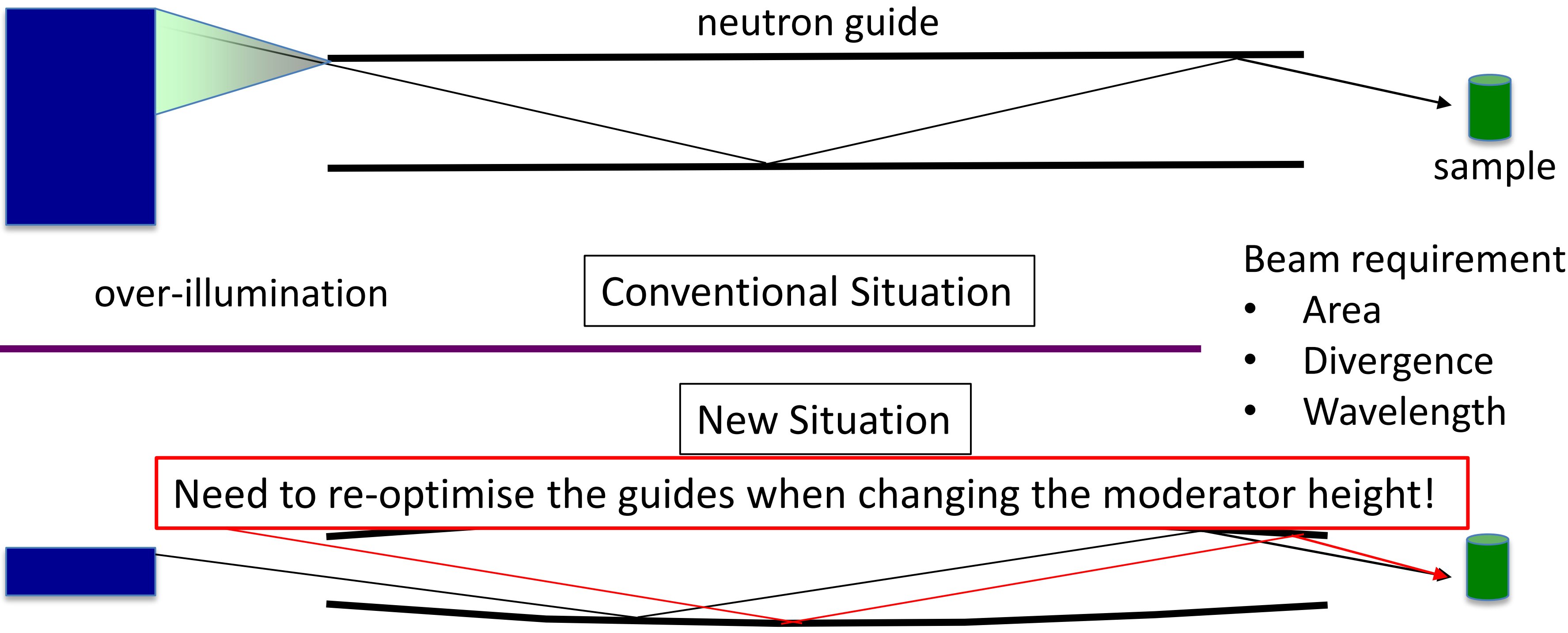
under-illumination

Beam requirements:
- Area
- Divergence
- Wavelength

=> less efficient brilliance transfer

Instrument performance:
Trade-off between increased Source Brightness and decreased Brilliance Transfer

# Guide Illumination



over-illumination

Conventional Situation

Beam requirements:
- Area
- Divergence
- Wavelength

New Situation

Need to re-optimise the guides when changing the moderator height!

under-illumination

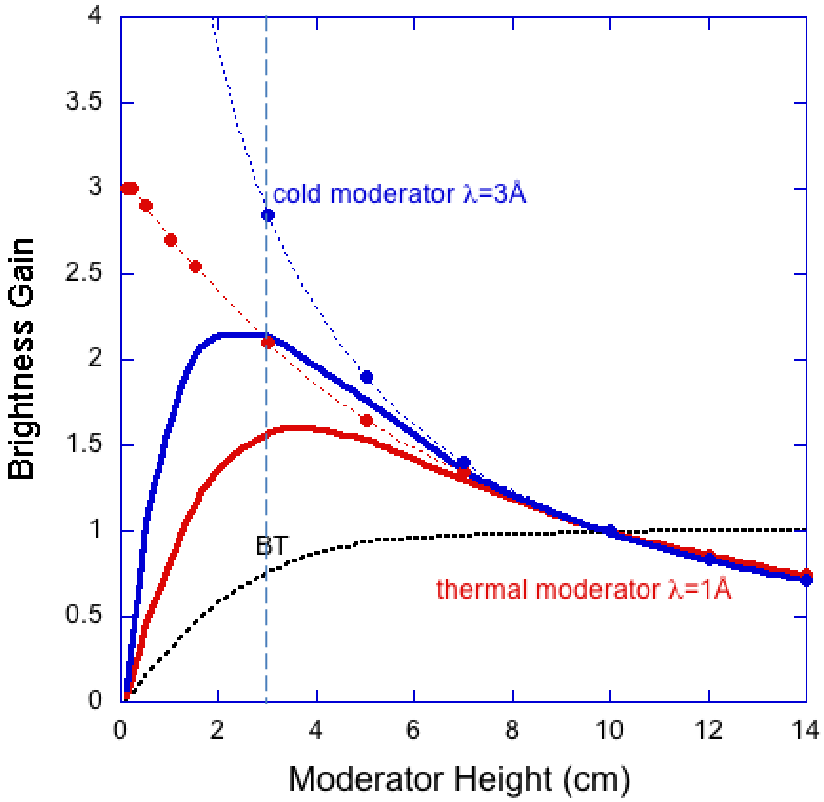
=> less efficient brilliance transfer

Instrument performance:
Trade-off between increased Source Brightness and decreased Brilliance Transfer

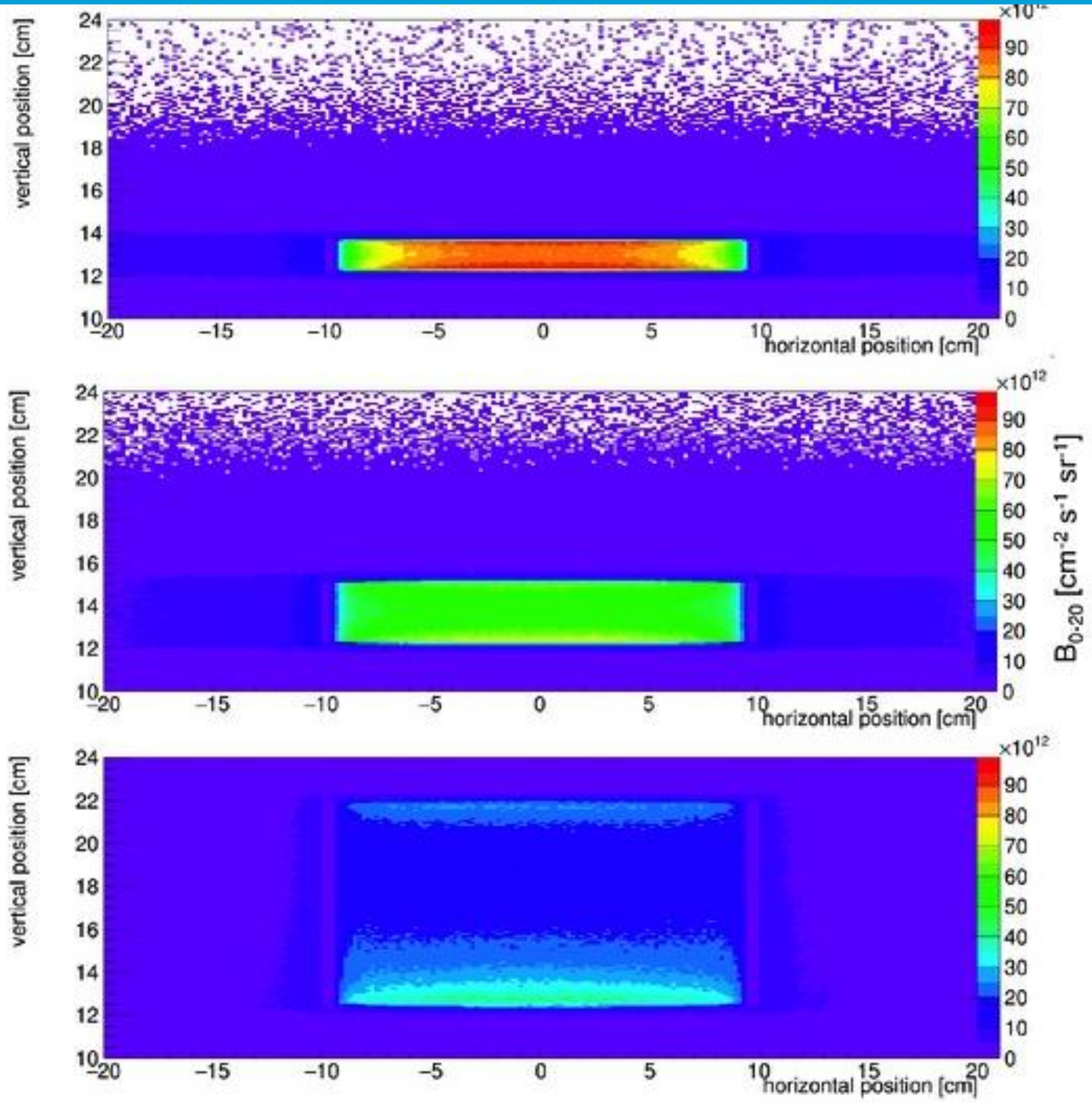
(K. Andersen)

# Optimal moderator height determined from brightness and brightness transport to the sample

3 cm chosen height



# Why flat moderators work

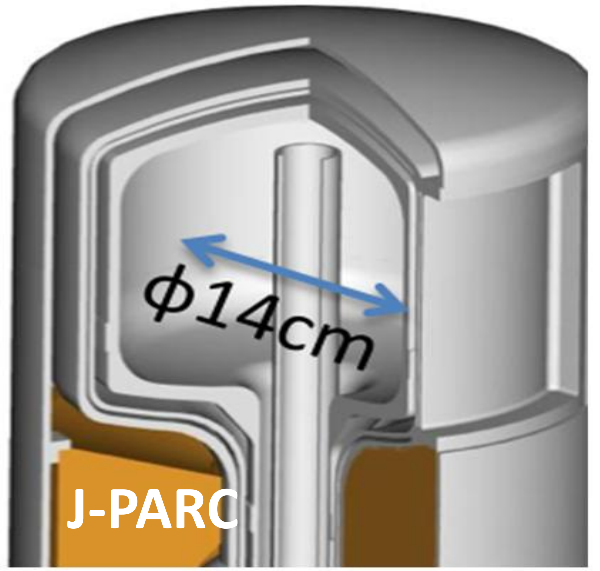


thermal neutrons arriving from the surroundings are transformed into cold ones within about 1 cm of the walls of the moderator vessel

along the direction of these walls this intense layer of cold neutrons can be seen from the outside into depths comparable to 10 cm.

Directional effect

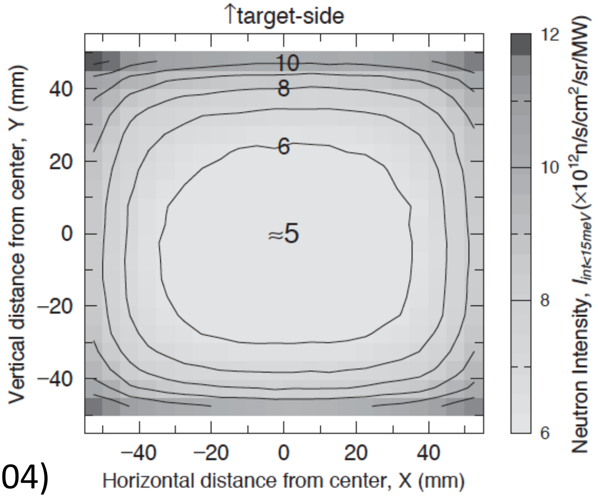
# Experimental confirmation at J-PARC of physics effects behind flat moderator concept



Brightness distribution of cold coupled moderator performed at MLF at J-PARC in 2015 by J-PARC-ESS team

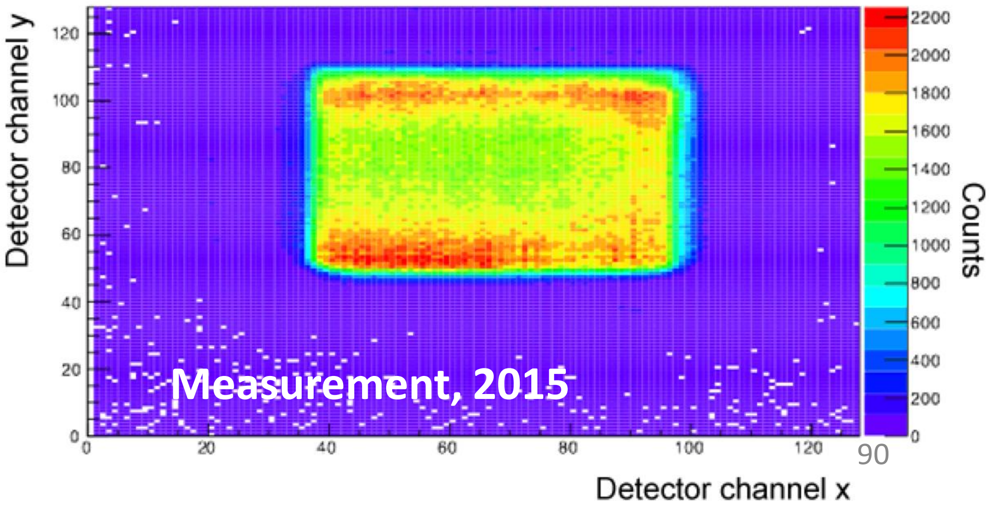
Results give full confirmation of the brightness distribution across the moderator: higher in target and reflector side (NIM Vol 903, 2018, page 38)

- Experimental confirmation of physics principles of flat moderators

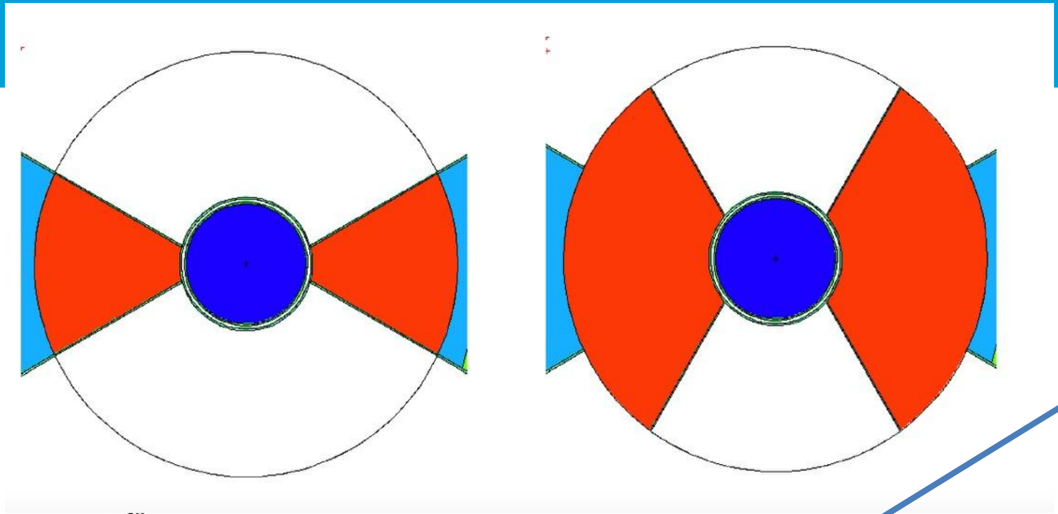


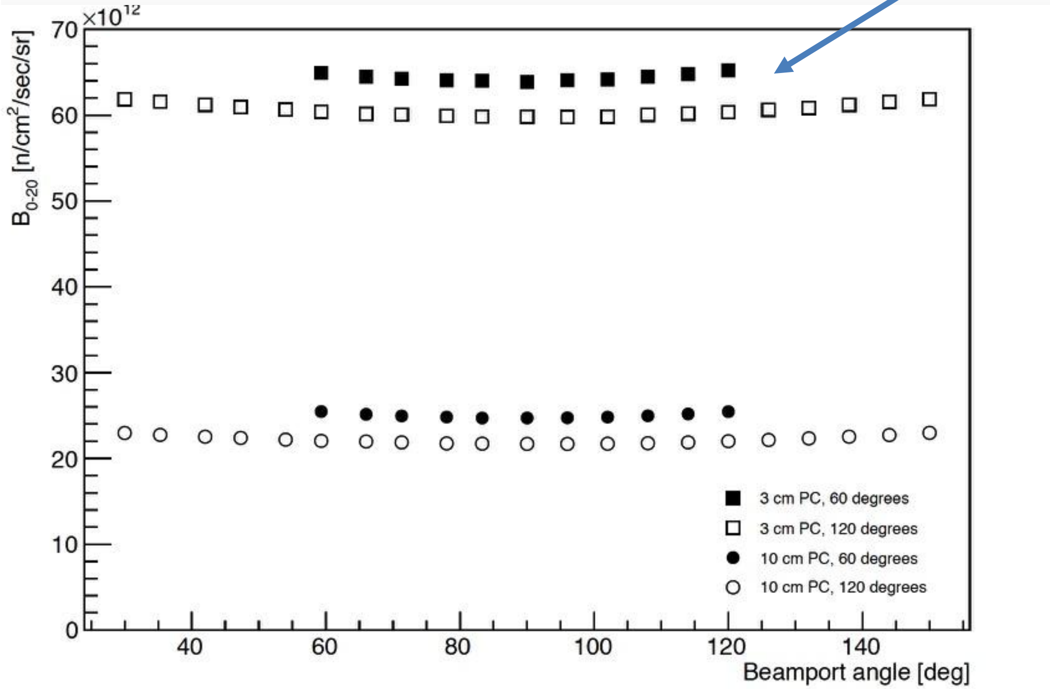
(Kai, 2004)

Brightness map of BL04 moderator at J-PARC



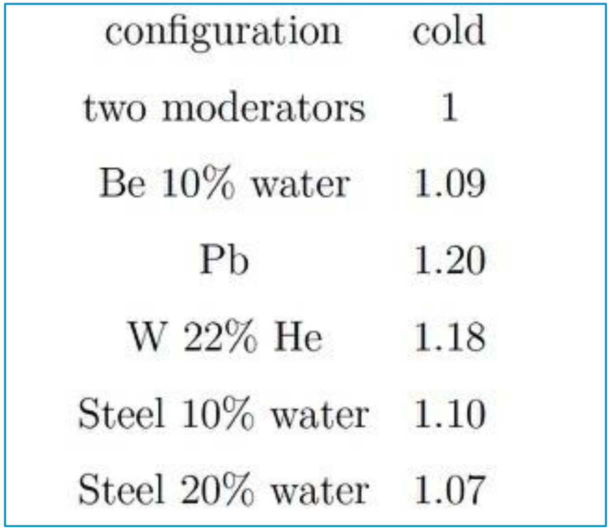
# A very important finding: only one flat moderator is needed





The small brightness difference could be easily compensated by a fast neutron reflector at the bottom

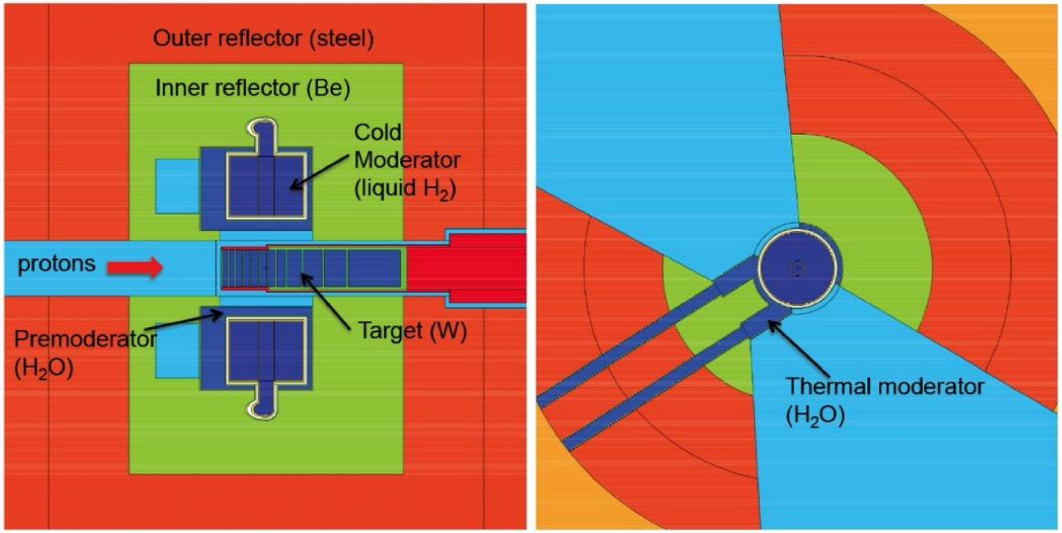
rel. increase



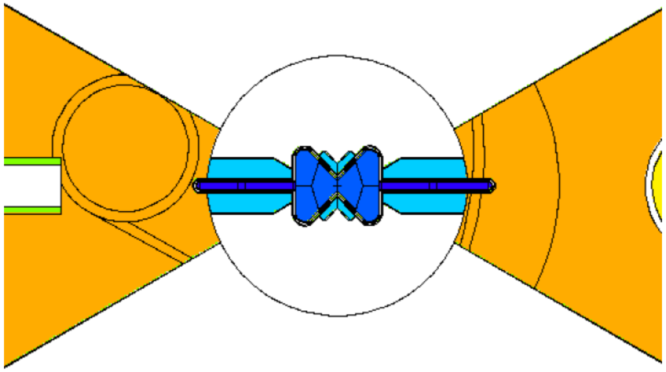
| configuration | cold |
|---|---|
| two moderators | 1 |
| Be 10% water | 1.09 |
| Pb | 1.20 |
| W 22% He | 1.18 |
| Steel 10% water | 1.10 |
| Steel 20% water | 1.07 |

# Impact on the design: number of moderators

TDR, 60 degree
openings, mandatory
two moderator systems
4 X 60 openings

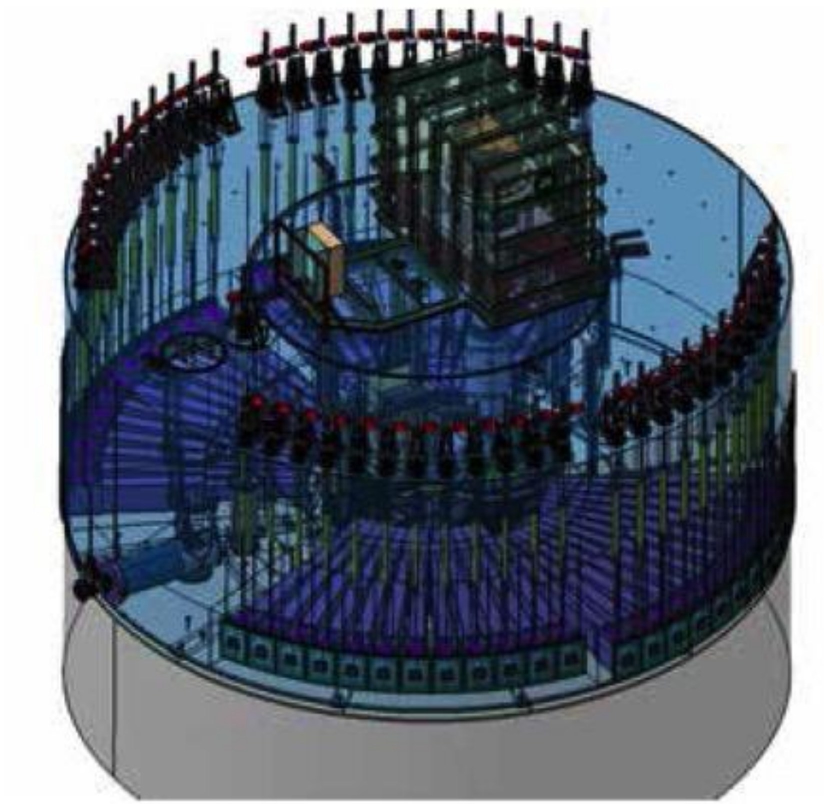


Possibility of a single moderator
System for 2 X 120 opening

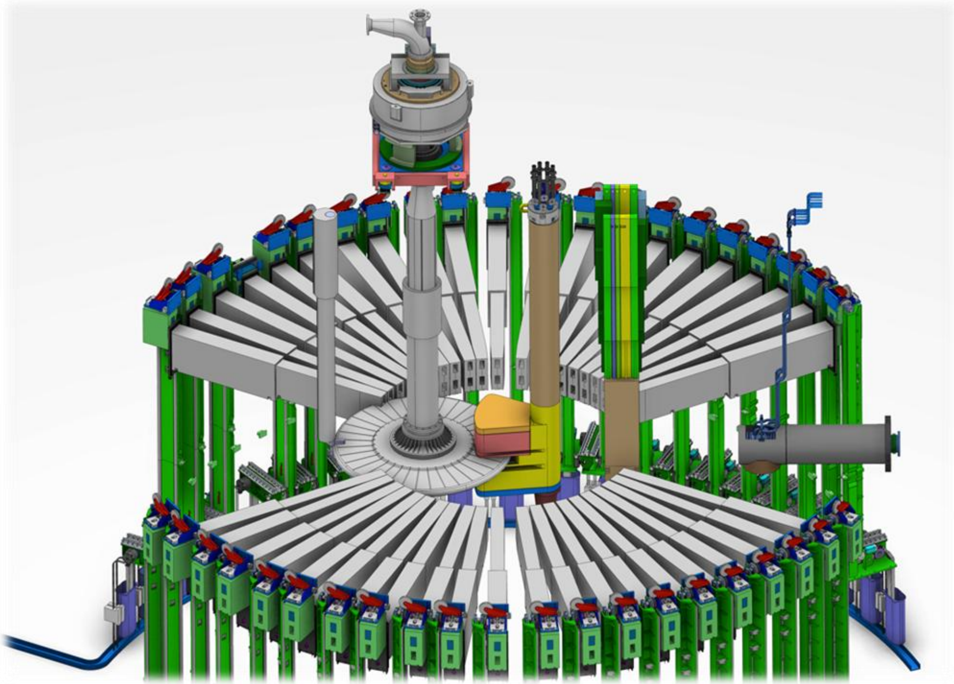


# Impact on the design: beam extraction

TDR



Present design

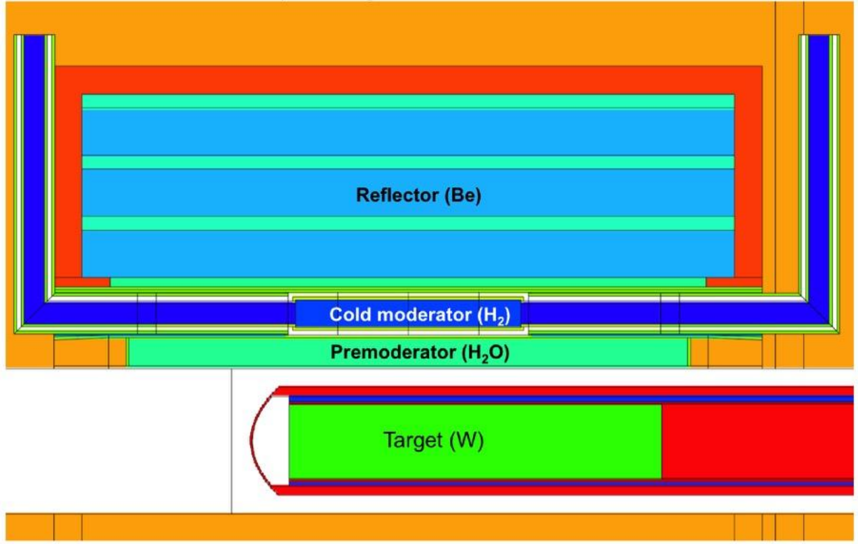


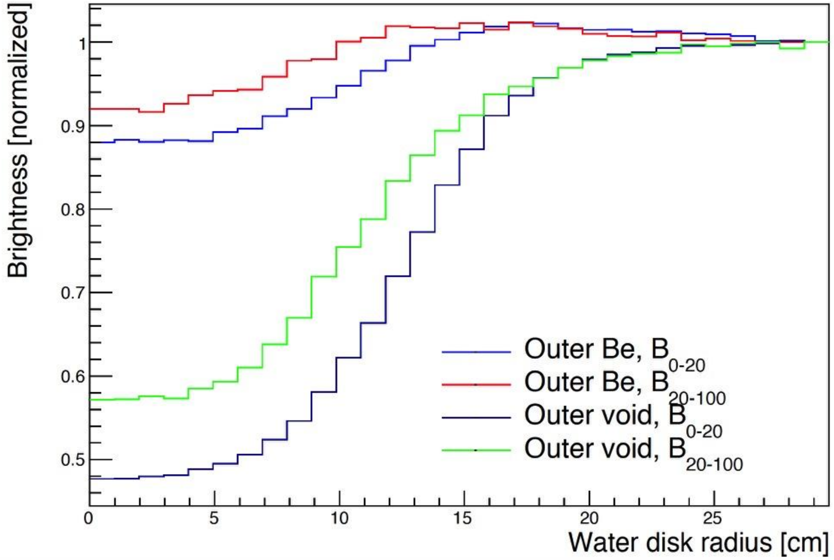
# Large premoderator for enhanced brightness

Shapes the neutron spectrum to feed the moderator with neutrons of the right energy (thermal)

Reduces the heat load on the cold moderator.

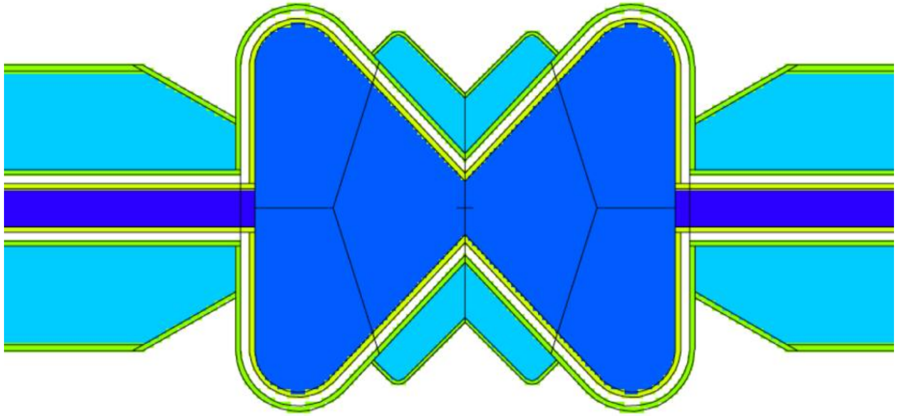
In the case of ESS geometry, a large premoderator increases the brightness.

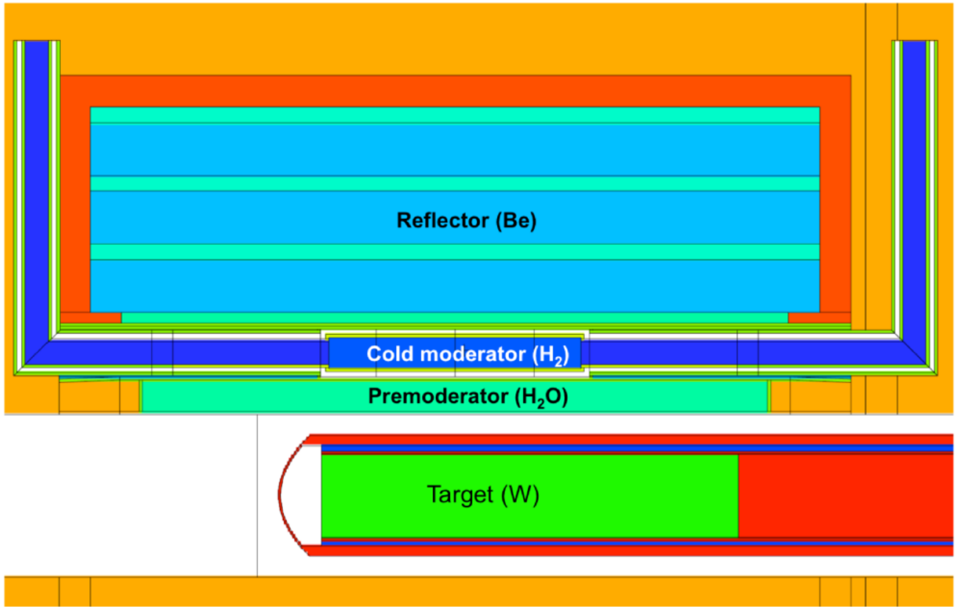


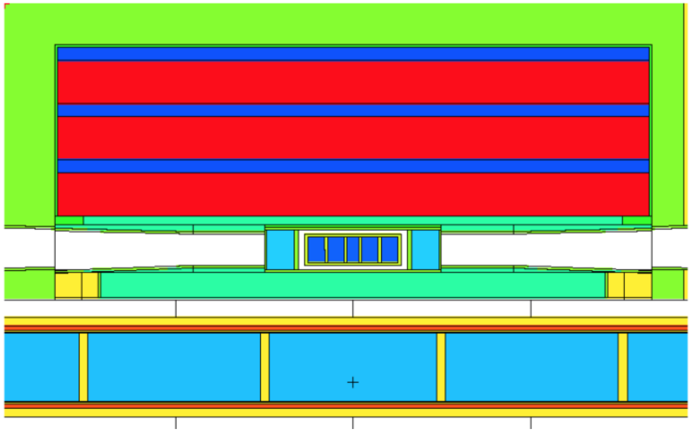


# “Butterfly” geometry gives the best design for:

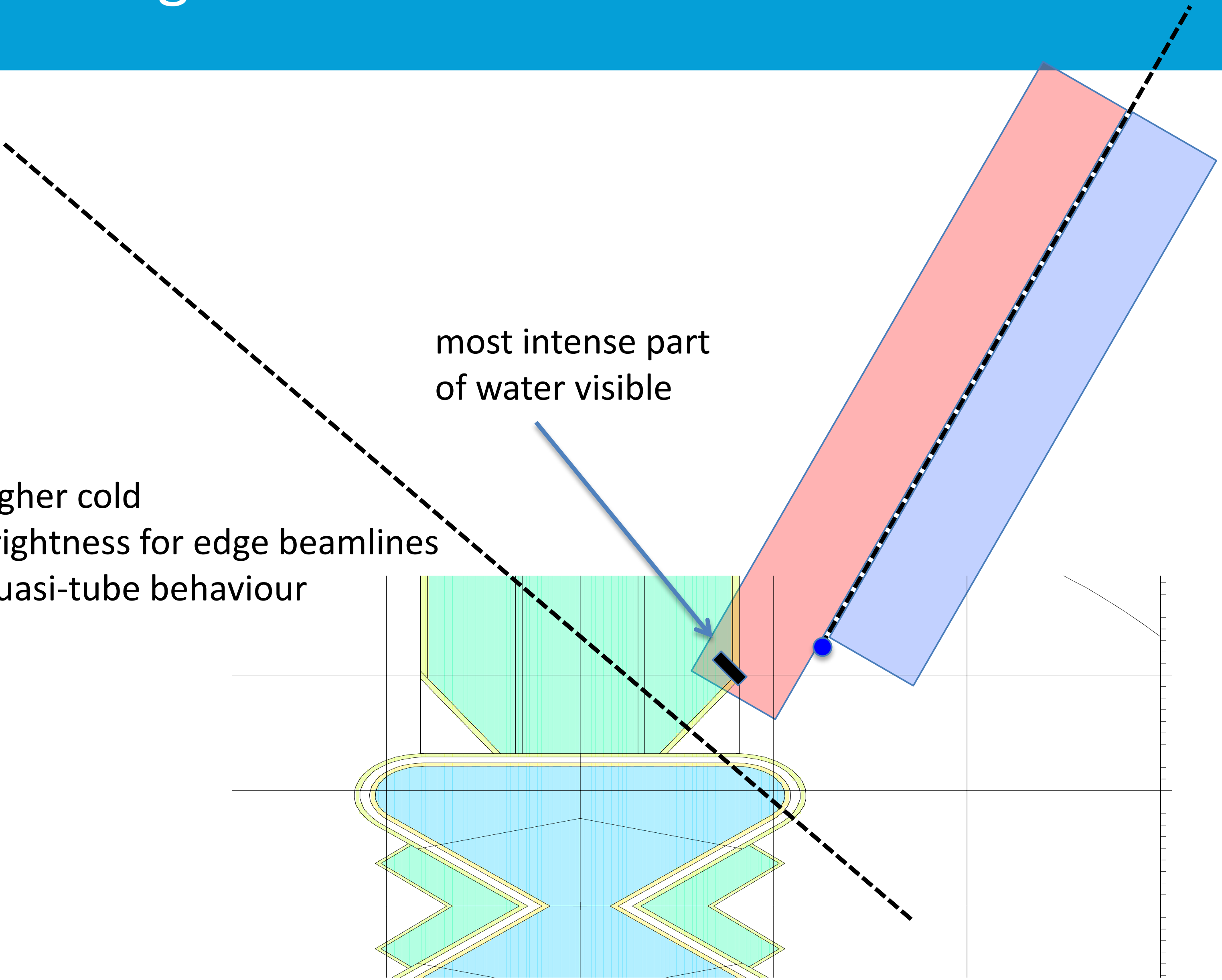
- ☐ Cover 2 × 120° sector uniformly
- ☐ 3 cm flat as selected with instruments
- ☐ Ease bispectral extraction
- ☐ High cold and thermal brightness in a single moderator







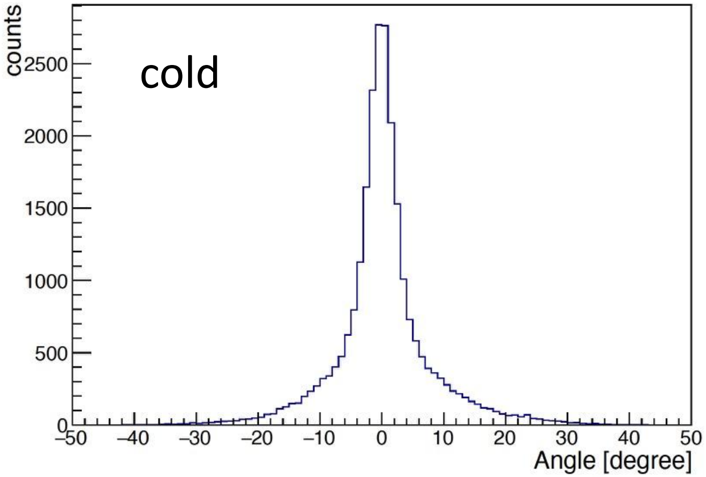
# Design features



most intense part
of water visible

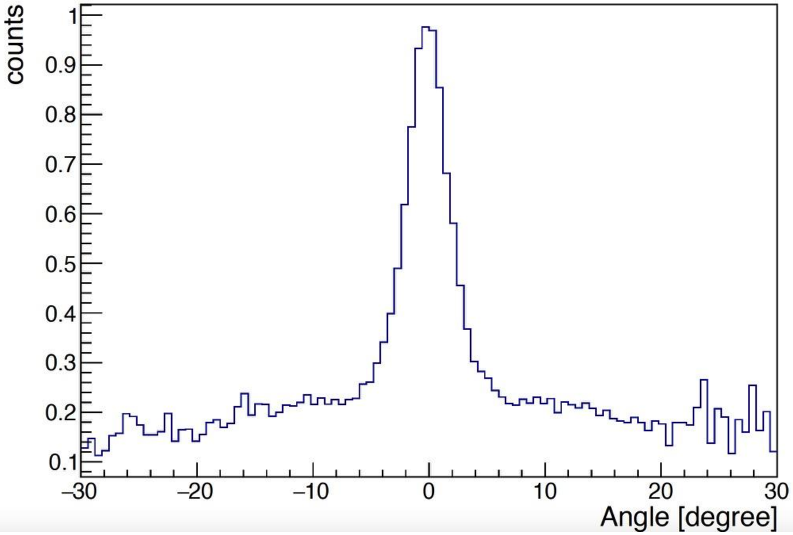
higher cold
brightness for edge beamlines
Quasi-tube behaviour

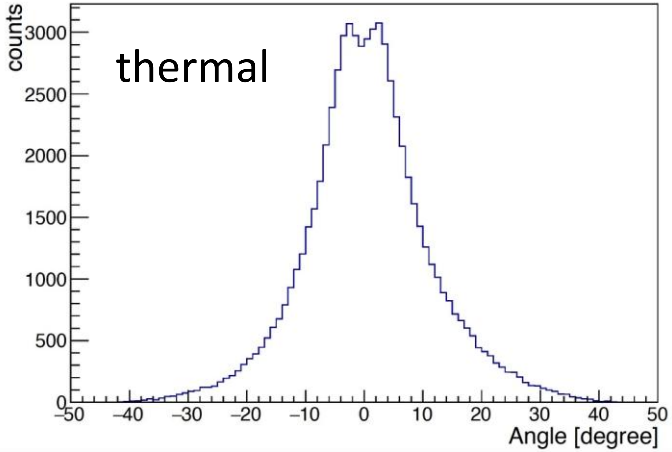
# Directionality!



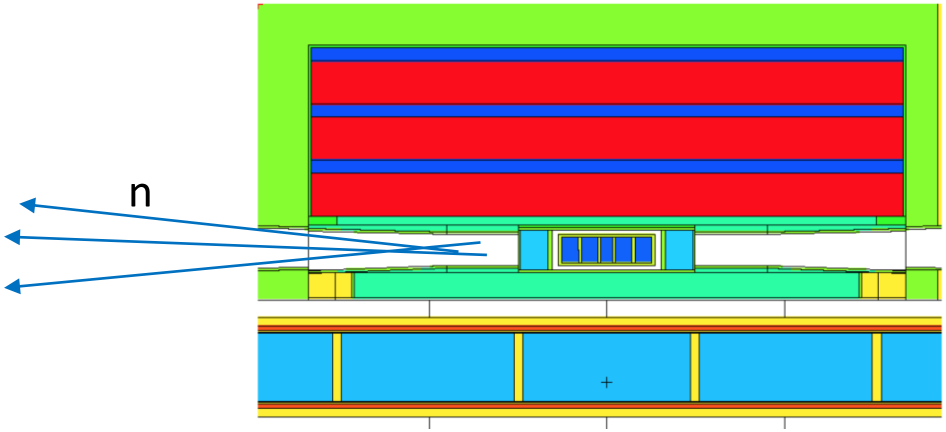
cold

Ratio cold/thermal

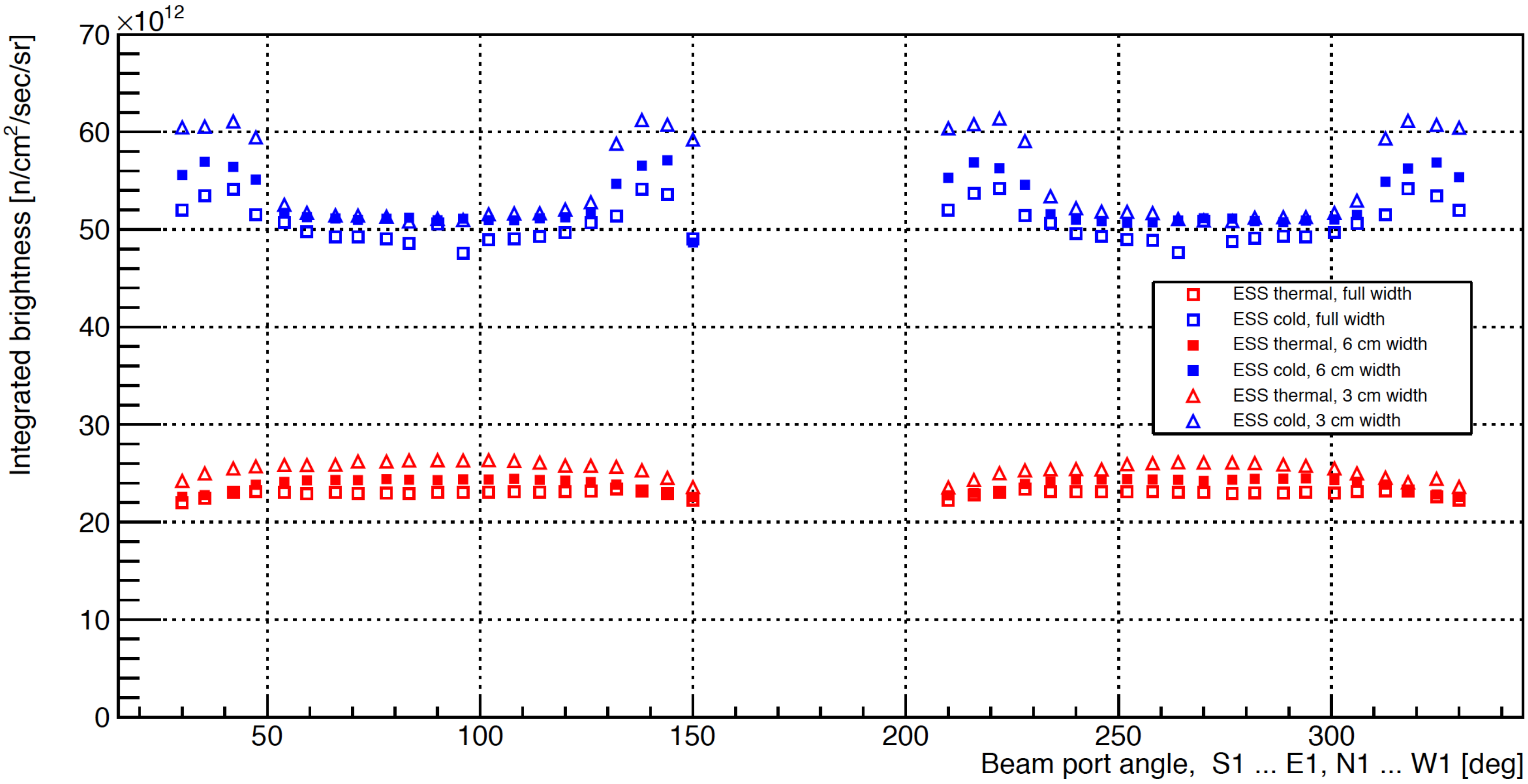




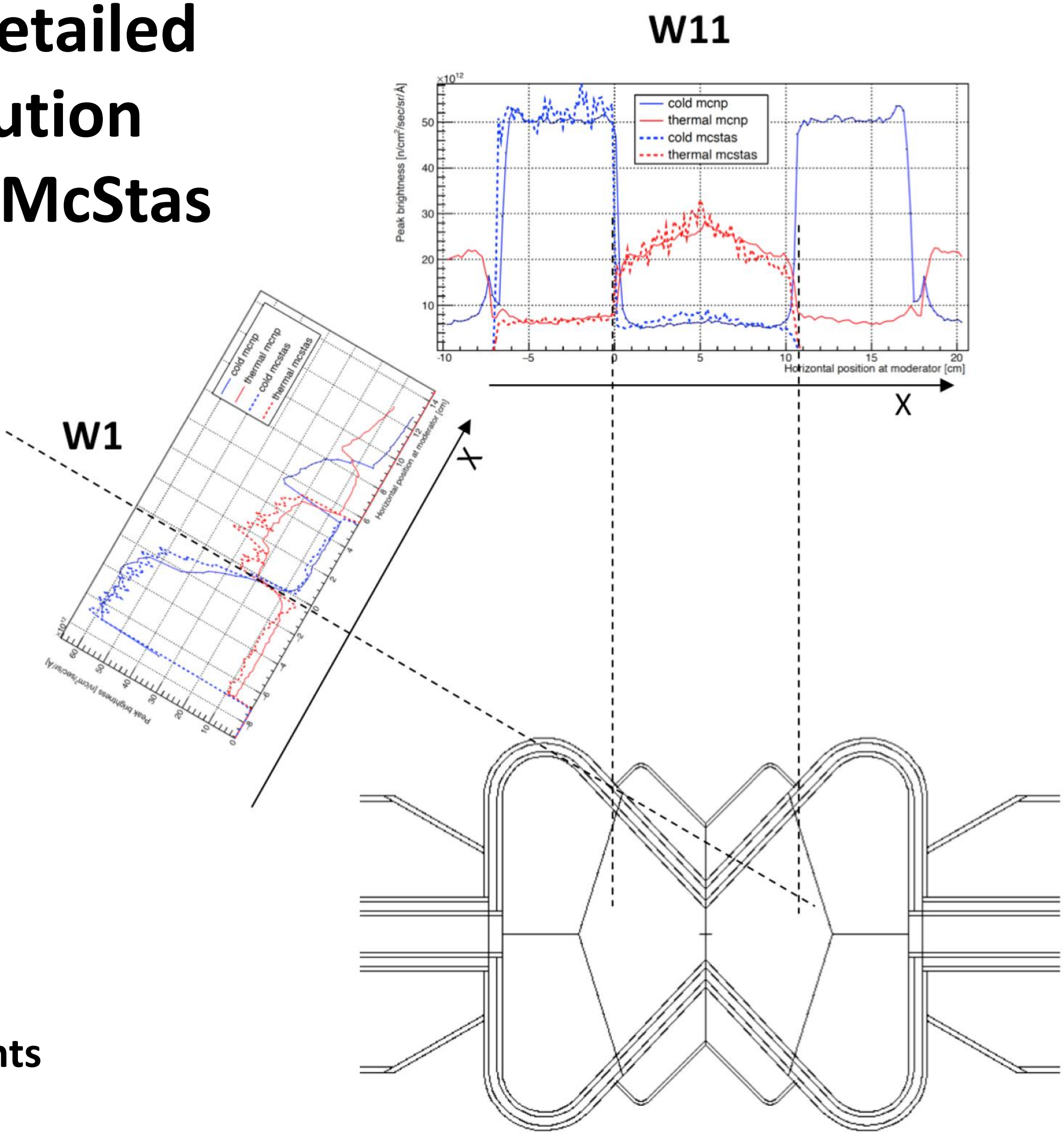
thermal



# Additional gain if < 6 cm width at the moderator is used (example NMX)



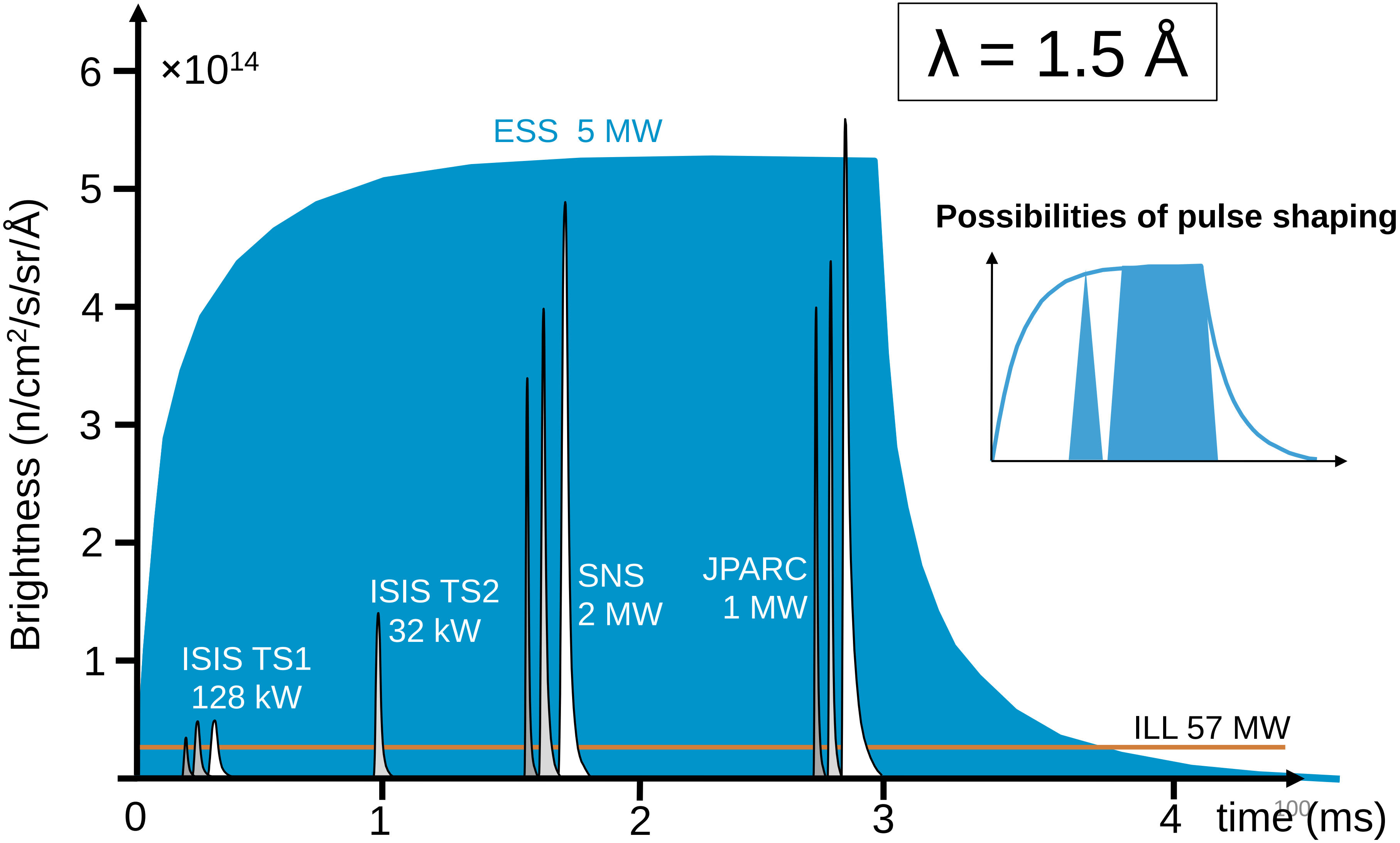
# Guide design can be optimized using detailed brightness distribution from MCNPX and McStas



- New McStas modules (P. Willendrup)
  - Detailed brightness distribution from moderator area
  - Analytical
  - Based on MCNP events

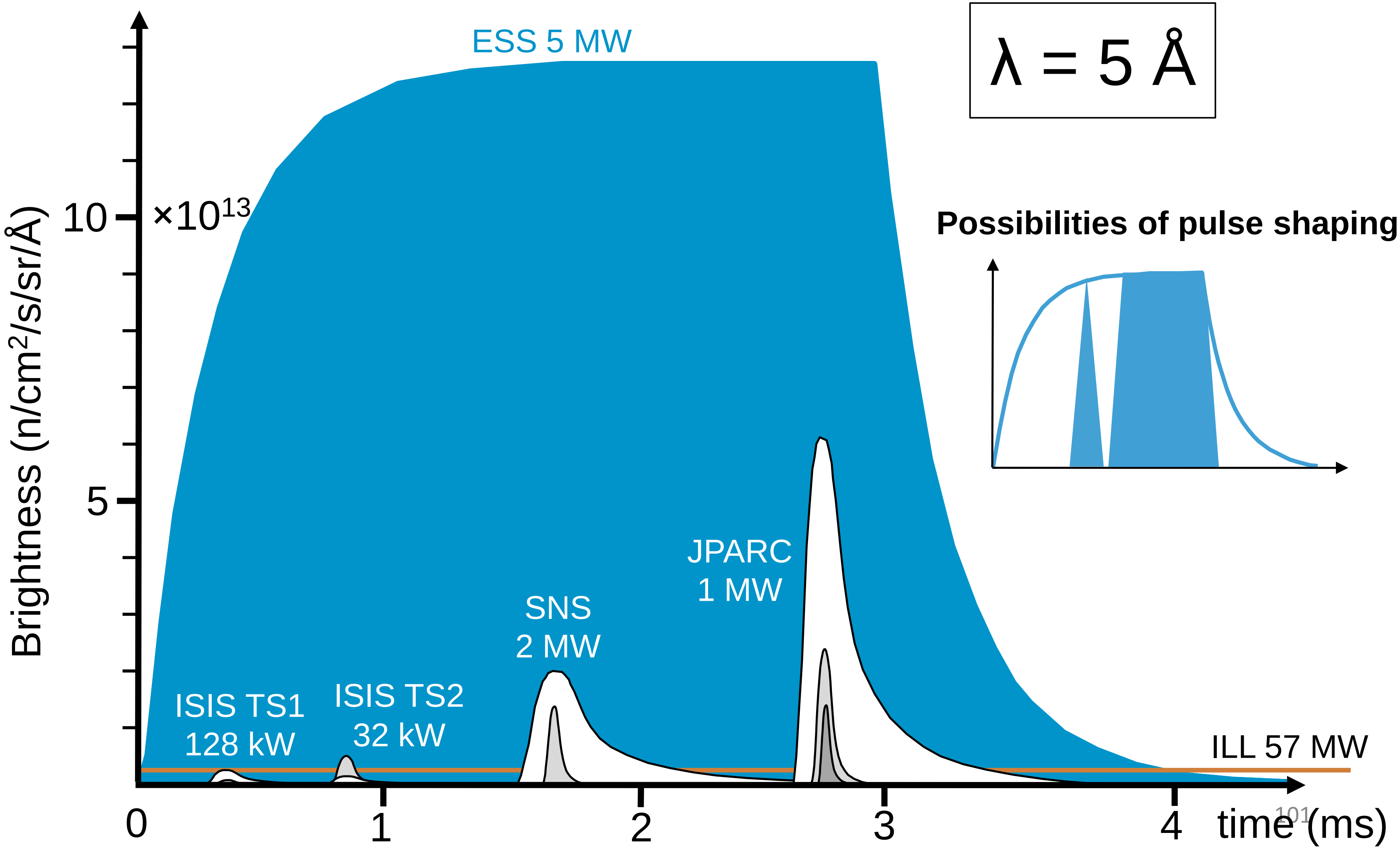
# Long-pulse performance

Version 25/4/2018



# Long-pulse performance

Version 25/4/2018

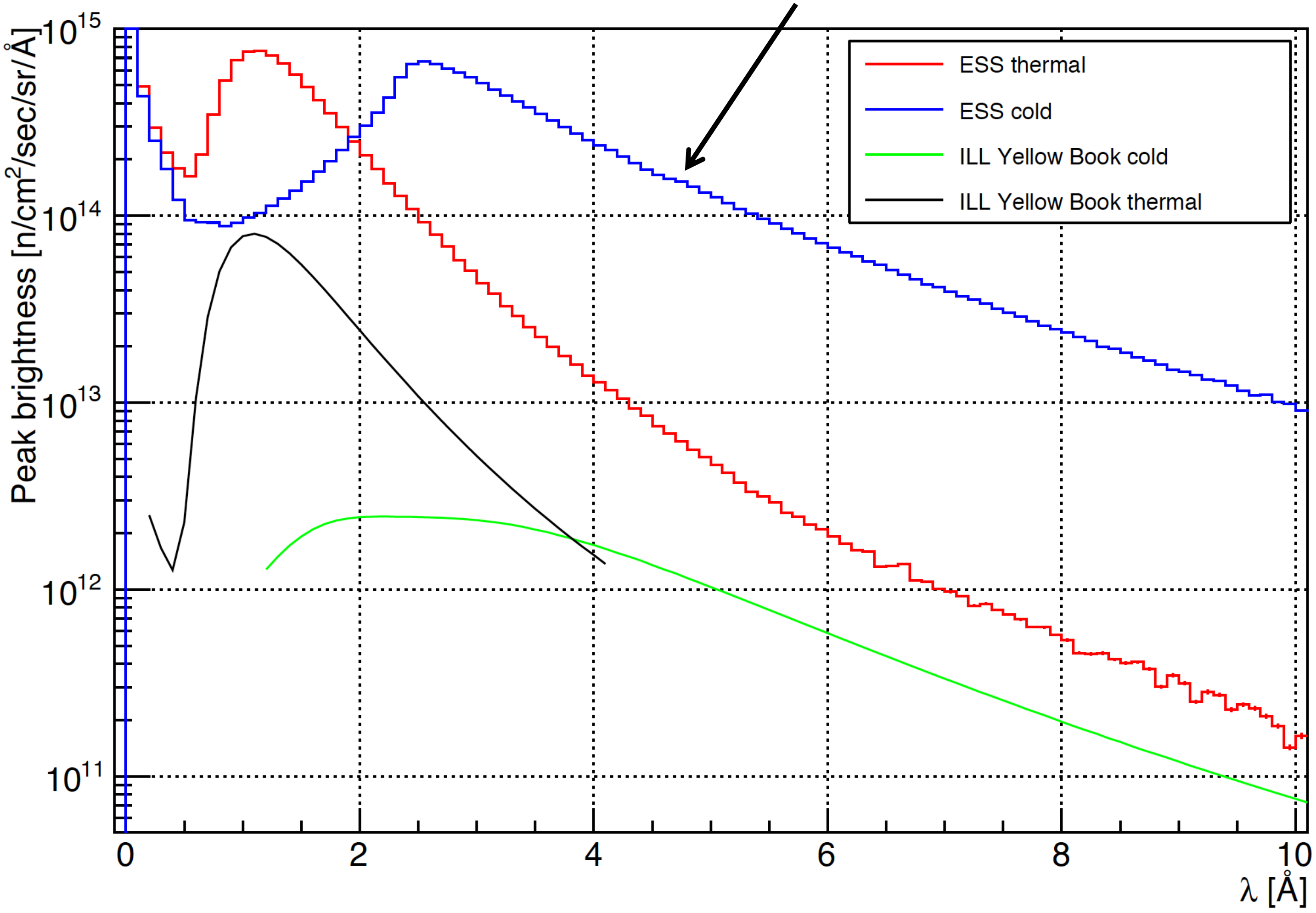


λ = 5 Å

**Possibilities of pulse shaping**

# Brightness spectra comparison with ILL

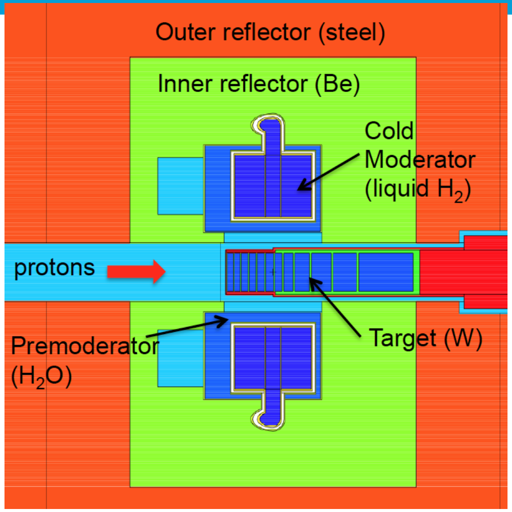
Average over 42 beamports

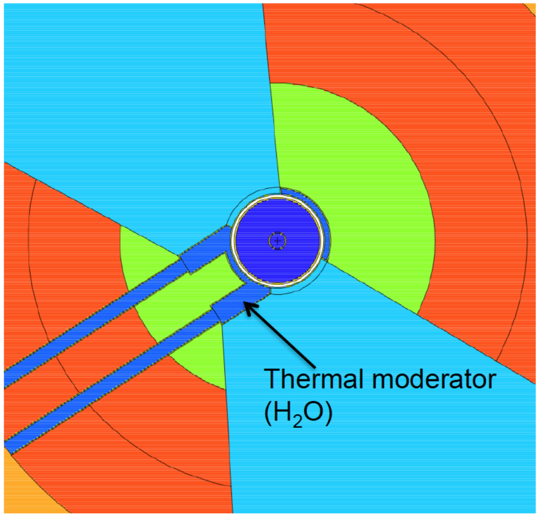


ILL Yellow book: Institut Laue-Langevin. `ILL Yellow Book 2008.' http://www.ill.eu/?id=1379 , 2008.

# six years long moderator design and decision process has come to an end…

- ☐ 2012-13: TDR volume moderators
  - ☐ Two identical high-intensity moderators above and below the target
  - ☐ 2X60 openings

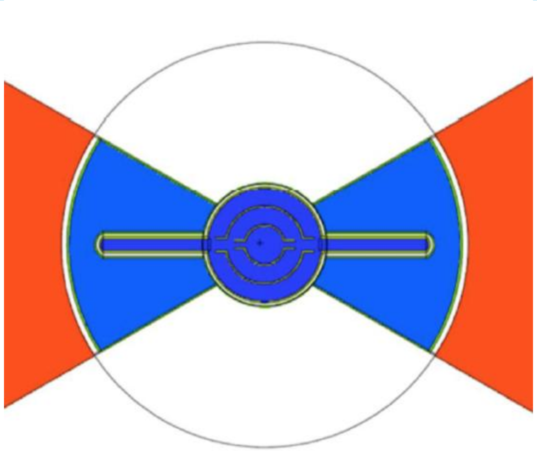


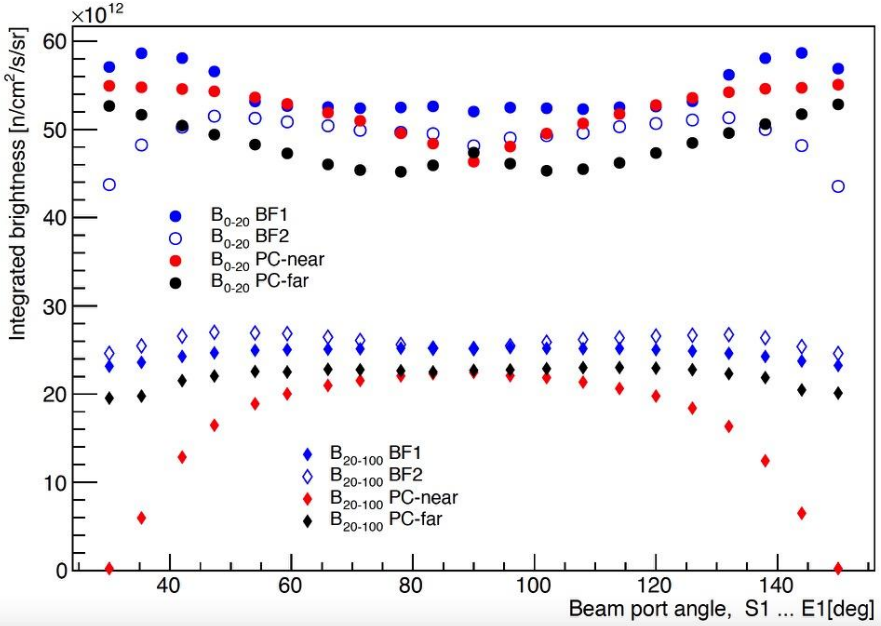


[ESS TDR, page 174]

# six years long moderator design and decision process has come to an end…

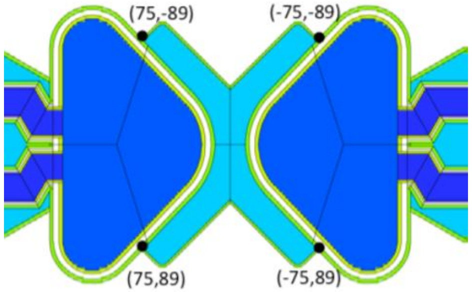
- 2012-13: TDR volume moderators
  - Two identical high-intensity moderators above and below the target
  - 2X60 openings
- 2014: Pancake moderator
  - Factor 2.5 in cold brightness
  - Difficult bispectral extraction
  - Several options considered for bottom moderator

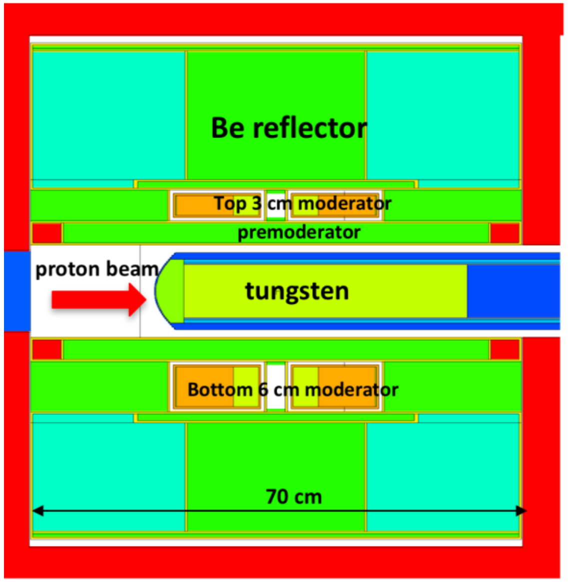




# six years long moderator design and decision process has come to an end…

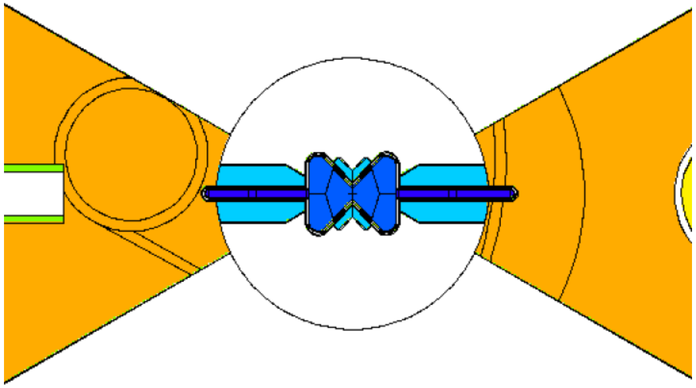
- 2012-13: TDR volume moderators
    - Two identical high-intensity moderators above and below the target
    - 2X60 openings
- 2014: Pancake moderator
    - Factor 2.5 in cold brightness
    - Difficult bispectral extraction
    - Several options considered for bottom moderator
- 2015: Butterfly BF2 moderator
    - Double-decker beam extraction in 2X120 sectors both above and below target
    - 3 cm on top, 6 cm on bottom
    - Higher thermal brightness than pancake

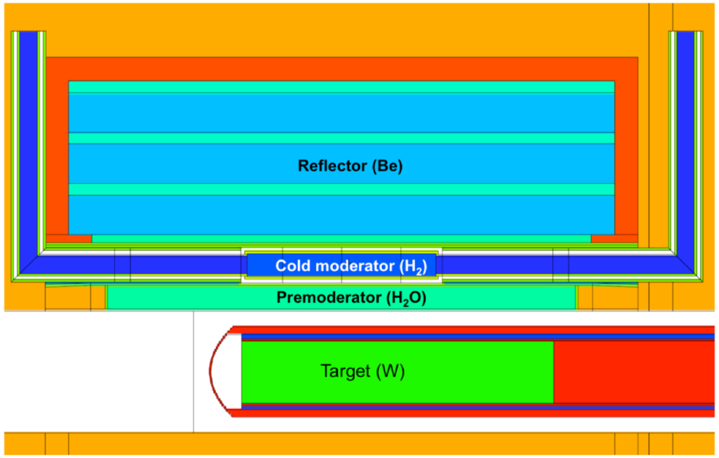




# six years long moderator design and decision process has come to an end…

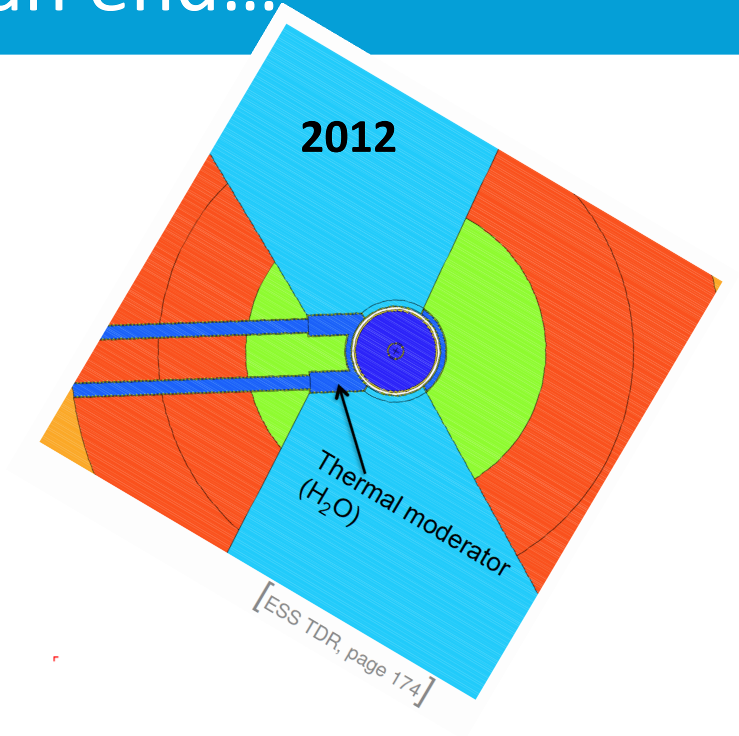
- 2012-13: TDR volume moderators
  - Two identical high-intensity moderators above and below the target
  - 2X60 openings
- 2014: Pancake moderator
  - Factor 2.5 in cold brightness
  - Difficult bispectral extraction
  - Several options considered for bottom moderator
- 2015: Butterfly BF2 moderator
  - Double-decker beam extraction in 2X120 sectors both above and below target
  - 3 cm on top, 6 cm on bottom
  - Higher thermal brightness than pancake
- 2016: Butterfly BF1 moderator
  - Maximum cold and thermal brightness
  - Better beam extraction
  - All instruments look at top moderator
  - Steel reflector at the bottom
  - Keep double decker, bottom moderator space available for future upgrades and novel ideas.





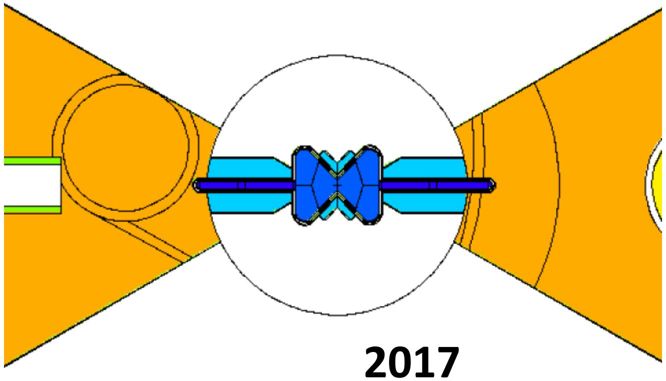
# six years long moderator design and decision process has come to an end…

- 2012-13: TDR volume moderators
  - Two identical high-intensity moderators above and below the target
  - 2X60 openings
- 2014: Pancake moderator
  - Factor 2.5 in cold brightness
  - Difficult bispectral extraction
  - Several options considered for bottom moderator
- 2015: Butterfly BF2 moderator
  - Double-decker beam extraction in 2X120 sectors both above and below target
  - 3 cm on top, 6 cm on bottom
  - Higher thermal brightness than pancake
- 2016: Butterfly BF1 moderator
  - Maximum cold and thermal brightness
  - Better beam extraction
  - All instruments look at top moderator
  - Steel reflector at the bottom
  - Keep double decker, bottom moderator space available for future upgrades and novel ideas.



**2012**

[ESS TDR, page 174]



**2017**

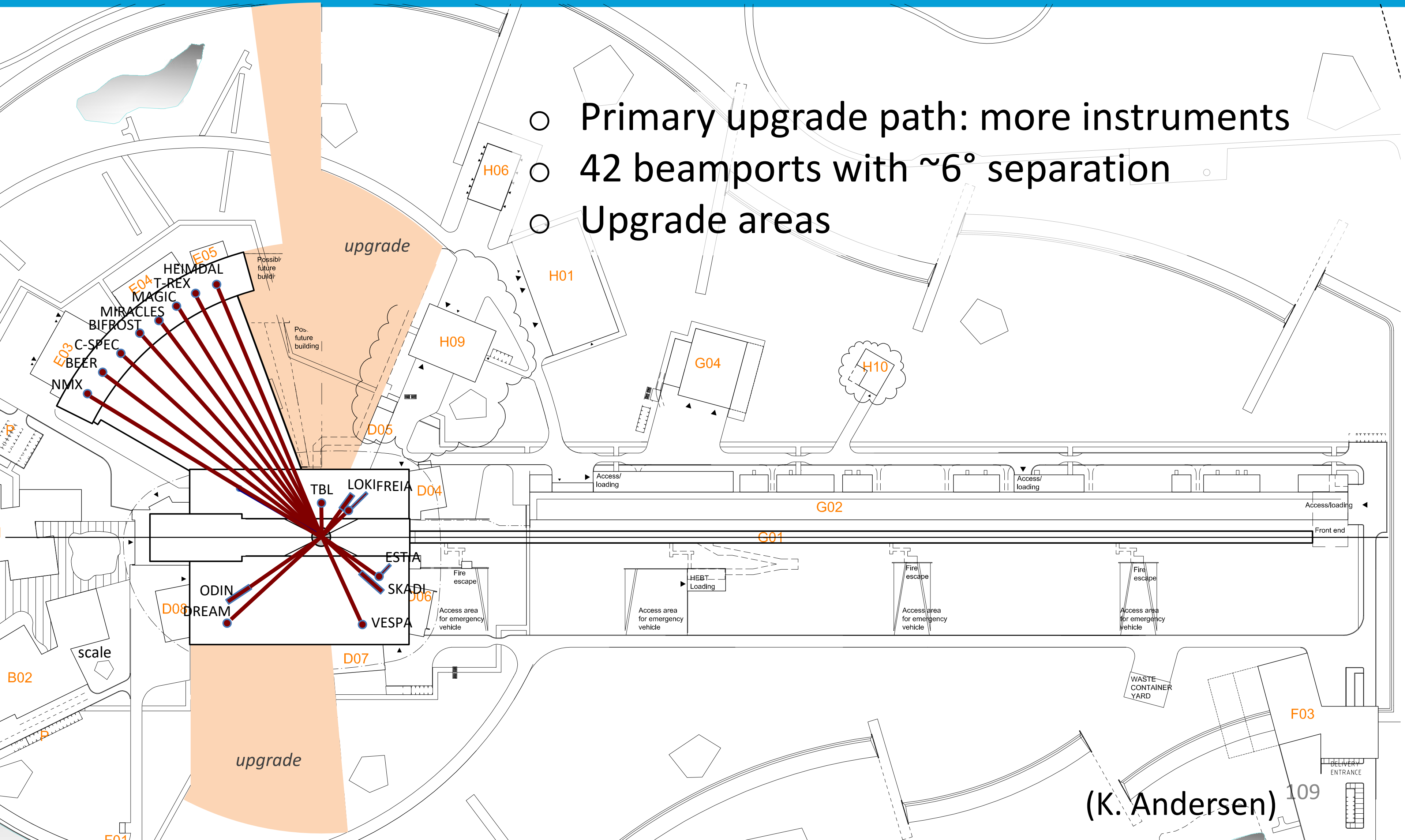
# Plans of low-dimensional moderators in the world

- ESS
- SNS TS2
- Upgrade Budapest reactor
- High Brilliance Source (Jülich)
- …

ESS cold moderator halves milled from two solid AL6061-T6 work pieces (Y. Baessler)

# Upgradeability

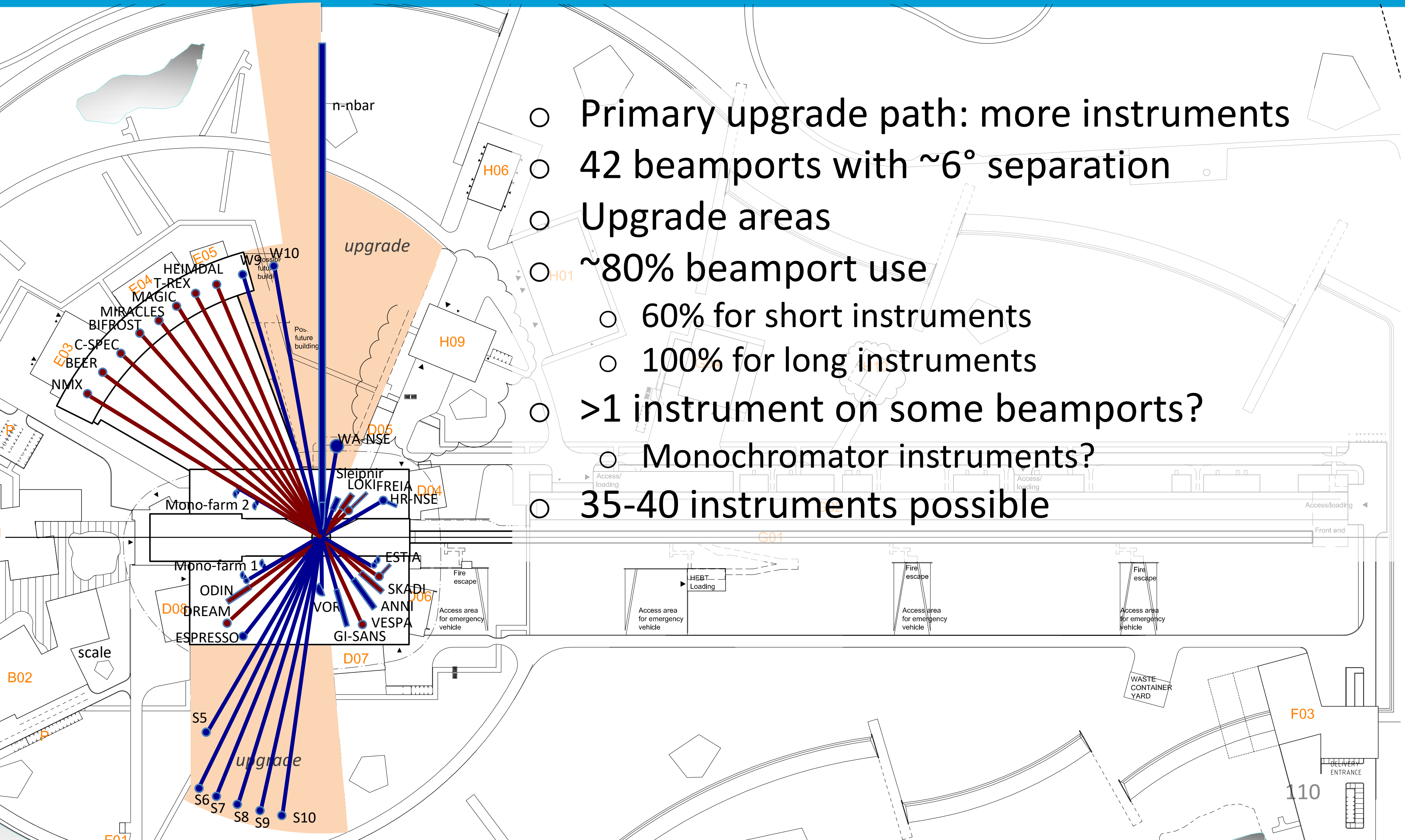
- Primary upgrade path: more instruments
- 42 beamports with ~6° separation
- Upgrade areas



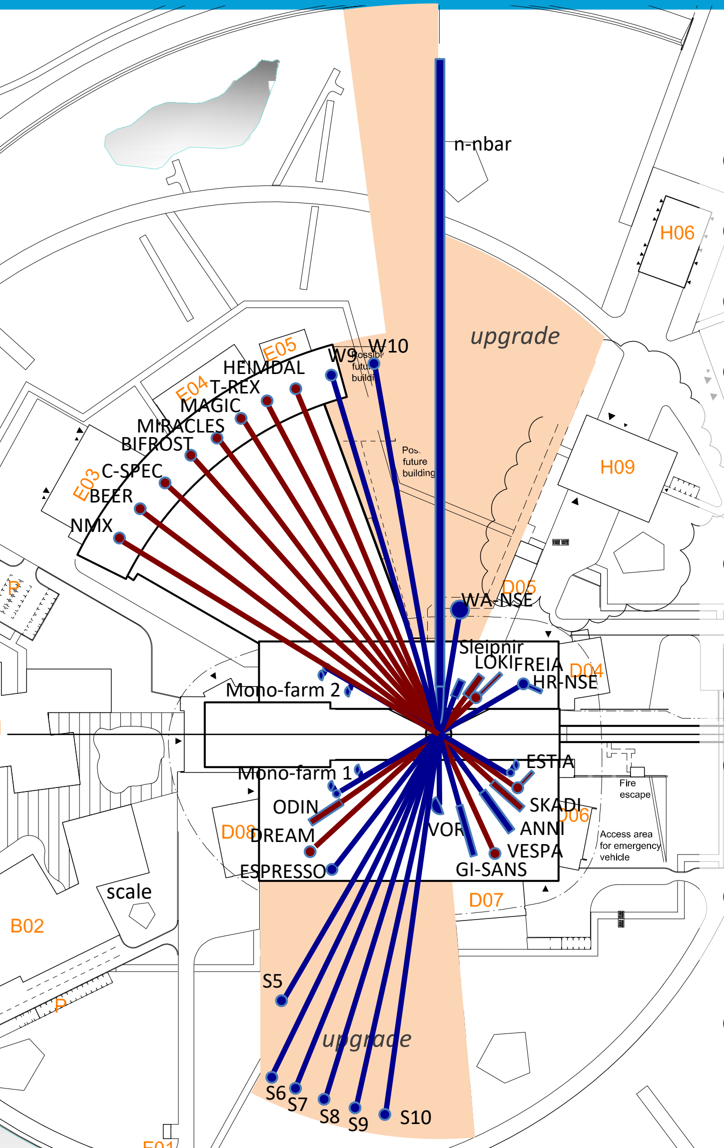
(K. Andersen)

# Upgradeability

- Primary upgrade path: more instruments
- 42 beamports with ~6° separation
- Upgrade areas
- ~80% beamport use
  - 60% for short instruments
  - 100% for long instruments
- >1 instrument on some beamports?
  - Monochromator instruments?
- 35-40 instruments possible



# Upgradeability



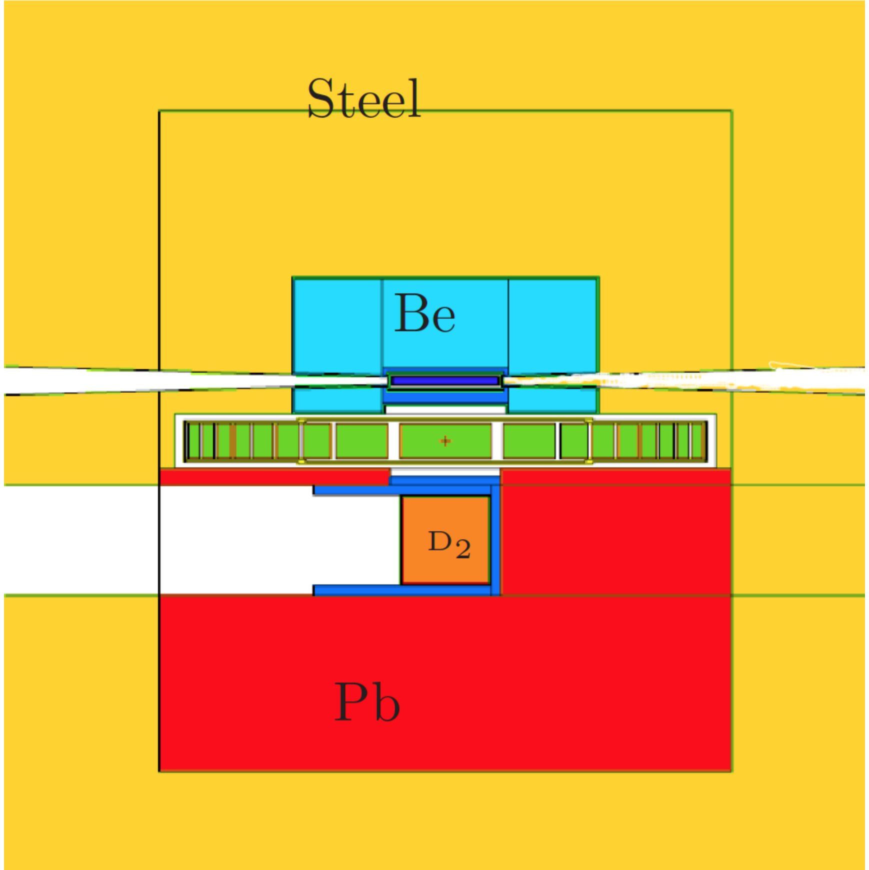
- Primary upgrade path: more instruments
- 42 beamports with ~6° separation
- Upgrade areas
- ~80% beamport use
  - 60% for short instruments
  - 100% for long instruments
- >1 instrument on some beamports?
  - Monochromator instruments?
- 35-40 instruments possible
- Lower moderator not yet defined
  - all beamports can view both moderators
- All beamports allow cold and/or thermal spectrum
- Freely tunable wavelength resolution
  - adapt resolution to experimental needs

# The available space for the bottom moderator should be used for *something good at something different*

- **Some possibilities**:
- High-intensity $D_2$ moderator for e.g. fundamental physics (nnbar)
- Extreme brightness moderator (e.g. small cross section tube moderator) for only a few beam lines
- UCN or VCN moderator
- Some of these solutions are not incompatible with a fast neutron reflector to further increase the brightness of the top moderator.

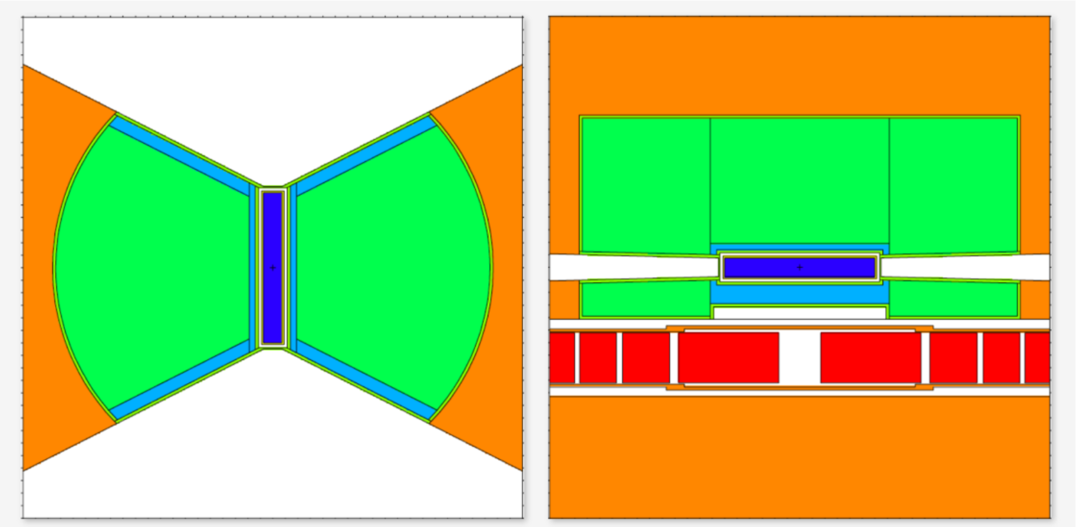
# Example: nnbar

- ☐ High-intensity $D_2$ moderator for e.g. fundamental physics (nnbar)
- ☐ Factor 3 gain in intensity
- ☐ Neutron-antineutron oscillation experiment
- ☐ Large international collaboration
- ☐ Letter of intent - 2015

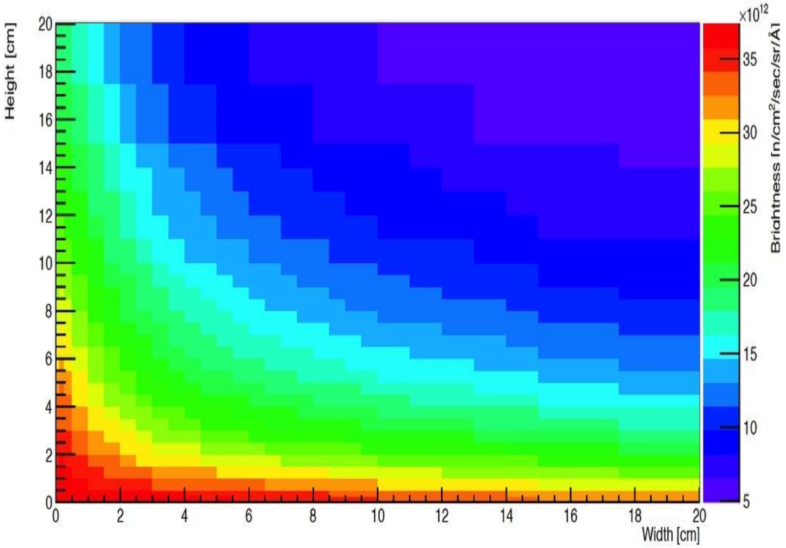


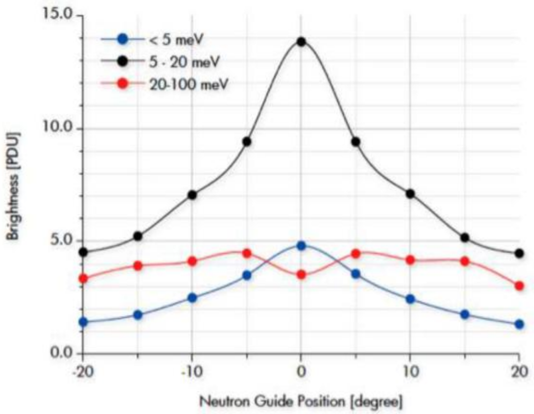
https://arxiv.org/pdf/1401.6003.pdf

# Example: tube moderators



(A. Takibayev, ICANS XXI, 2014)

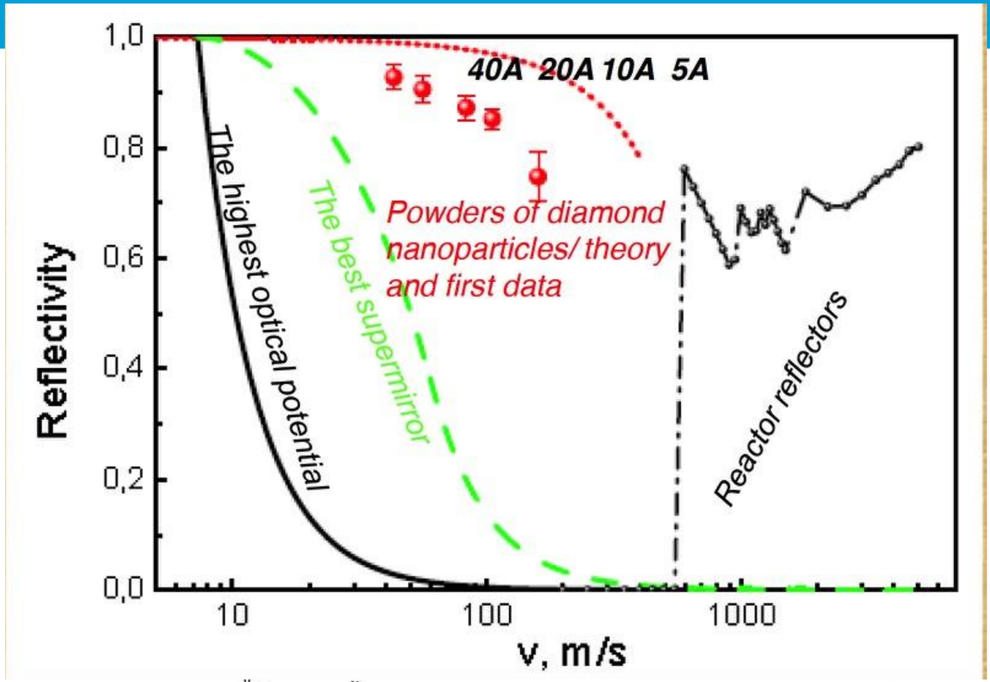




**Directionality:**
**1.5 cm x 1.5 cm tube moderator**

# Example: use of nanodiamonds to enhance Very Cold Neutrons

- Wavelength of VCN comparable to the size of nanodiamonds (about 4 nm)
- Possibility of reflection of VCN.
  - Quasi specular reflection of cold neutrons
  - Total reflection for very cold neutrons
- Problem of contamination of hydrogen: neutron absorption.
  - Fluorination removes $H_2$.



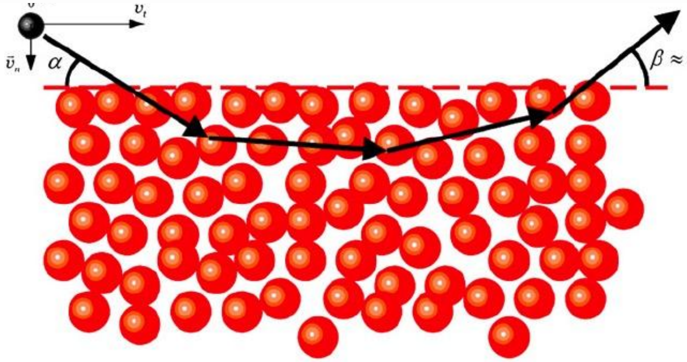


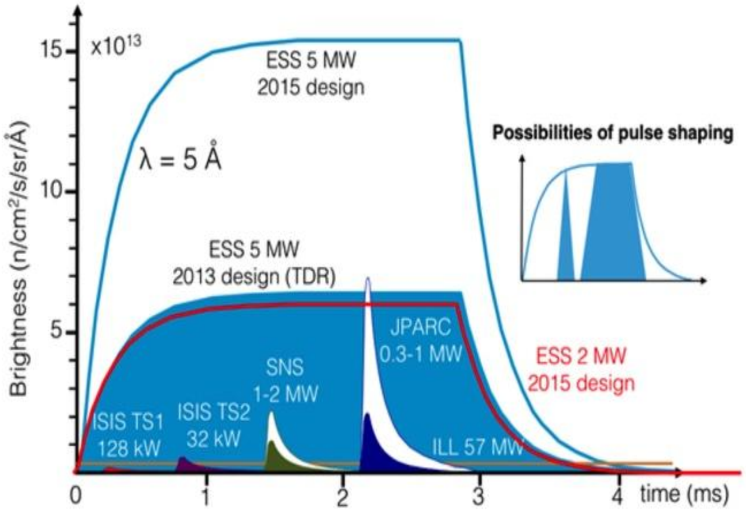
**Fig. 1.** Sketch of quasi-specular reflection of a cold neutron from powder of nanoparticles.

(V. Nesvizhevsky)

# In summary

- Moderator design had a major impact on the overall facility design (and it should):
  - Only one moderator for the initial instrument suite
  - Preserve the possibility to extract neutrons from above and below the target
  - Major upgrade possibilities
  - Beam extraction and moderator geometry adapted in an iterative process study

At 2 MW the original goal of the 2013 TDR design is achieved.



- <u>The facility design was driven by the physics properties of the moderators</u>

# *Thank you for your attention*