

---

ICTP, 21.10.05

# Optimization of source performance

F. Mezei  
HMI, Berlin & Los Alamos National Laboratory

---

ICTP, 21.10.05

# Optimization of source performance for neutron scattering experiments

F. Mezei

HMI, Berlin & Los Alamos National Laboratory

# Subjects

---

- **Ways to produce neutrons:  
the efficiency factor**
- **Global system requirements: contradictory needs of  
neutron scattering instruments**
- **Optimal performance: Peak flux theorem**
- **Global system requirements: neutron scattering  
needs vs. accelerator-target realities**
- **Long pulse concept: maximize peak and time  
average flux at the same time**
- **Conclusion**

# Ways to produce neutrons

---

## Energy balance: fast neutrons produced / joule energy (heat produced / energy consumed)

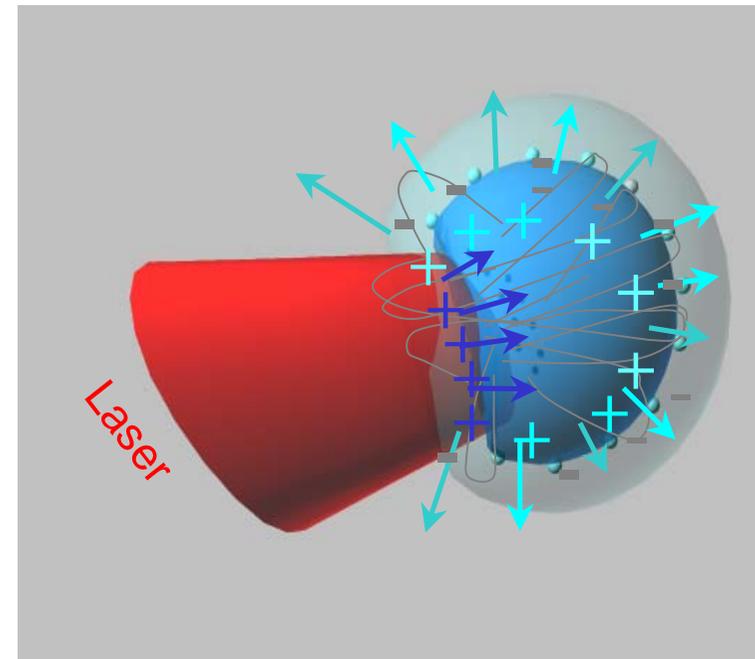
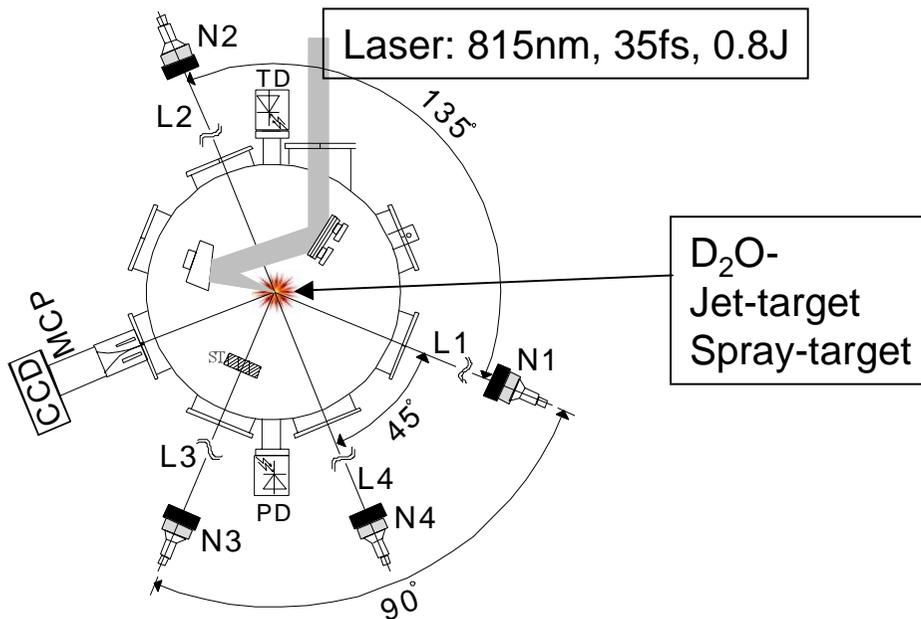
|                           |                |                                  |
|---------------------------|----------------|----------------------------------|
| Fission reactors:         | $\sim 10^9$    | (in $\sim 50$ liter volume)      |
| Spallation:               | $\sim 10^{10}$ | (in $\sim 1$ liter volume)       |
| Photo neutrons:           | $\sim 10^9$    | (in $\sim 0.01$ liter volume)    |
| Nuclear reaction (p, Be): | $\sim 10^8$    | (in $\sim 0.001$ liter volume)   |
| Laser induced fusion:     | $\sim 10^4$    | (in $\sim 10^{-9}$ liter volume) |

Also: Nature (Apr 2005): table top fusion by accelerating pyroelectric fields

## Spallation (0.5 – 5 GeV protons): best energetics

# One amazing example: table top neutron source

- **Nanoaccelerator by ultrashort, focussed laser pulse on  $20\ \mu\text{m}$   $\text{D}_2\text{O}$  droplet: relativistic light intensities.** Field-strength:  $1\ \text{MV}/\mu\text{m}$   
 $10^{19}\ \text{W}/\text{cm}^2$  power  $\rightarrow$  plasma  $\rightarrow$  deuterons accelerated to MeV  $\rightarrow$  **fusion !**  
Distribution of neutrons reveals plasma formation mechanism  
Laser driven  $\mu$ -size source of (fast) neutrons ( $\sim 10^4$  neutron/  $\sim 0.5\ \text{J}$  pulse)  
 $\text{d} + \text{D} \Rightarrow 3\text{He} (0.82\ \text{MeV}) + \text{n} (2.45\ \text{MeV})$ : Neutron – spectroscopy



# Development of neutron sources

---

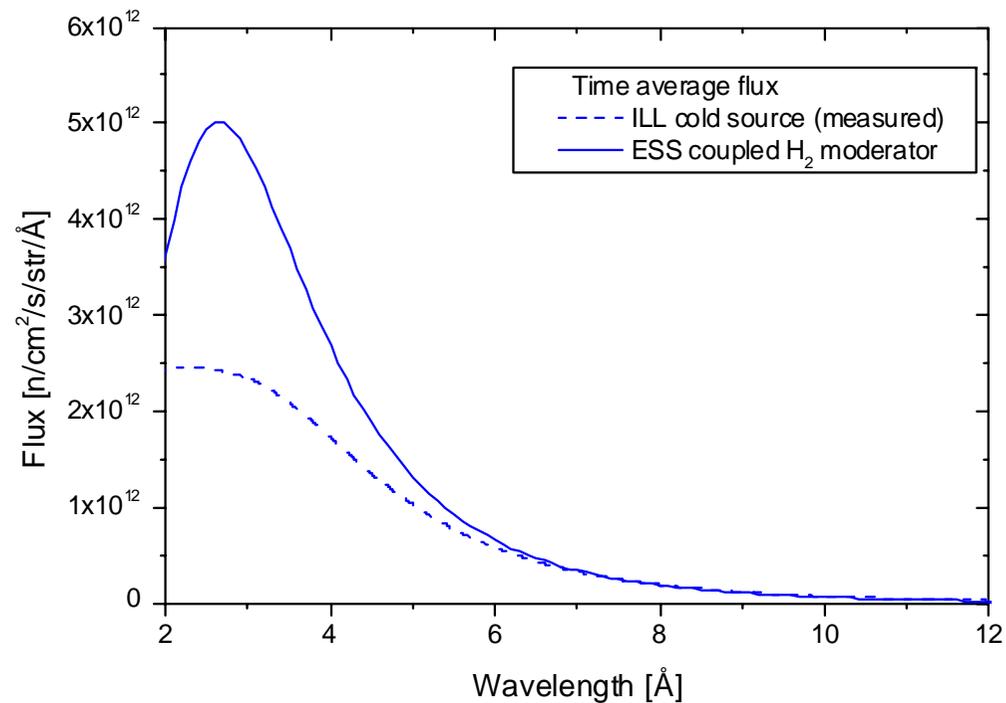
- **Parasitic use of energy research reactors**
- **Dedicated beam reactors (1958,.... )**
- **Pulsed spallation sources (1970's,... new facilities under construction):**
  - fewer neutrons more efficiently produced and used**
- **Next challenge in optimization:**
  - produce more neutrons and use them more efficiently**

# Efficiency gain by pulsed nature

---

5 MW spallation source:

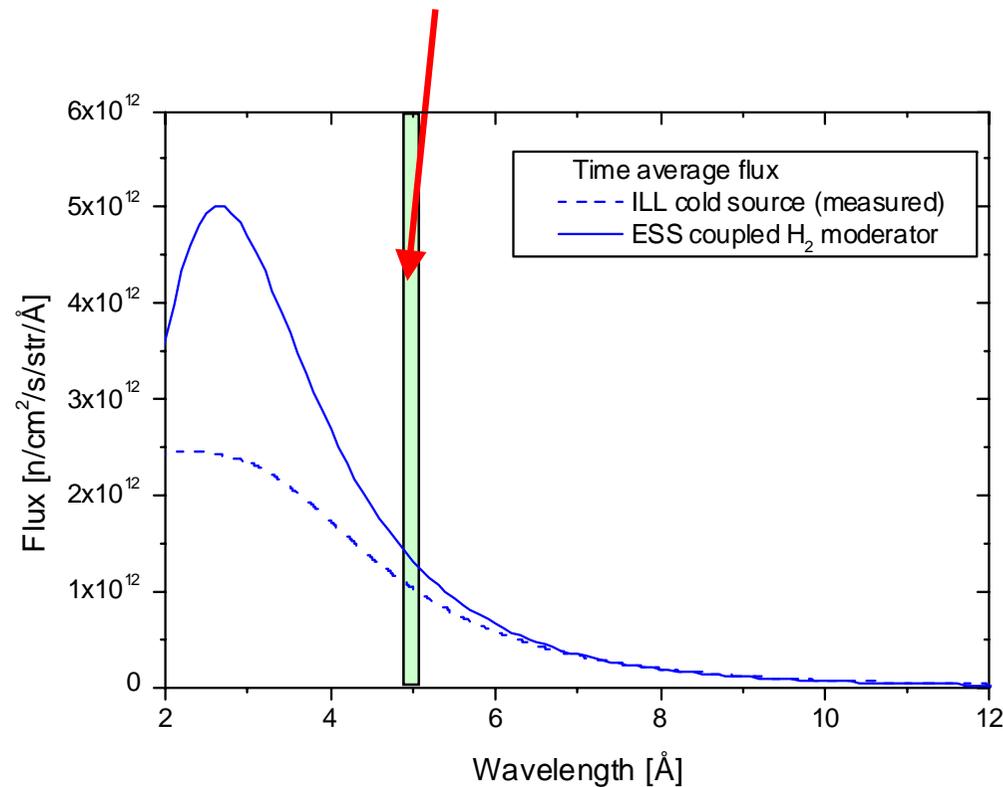
coupled cold moderator flux ~ ILL cold source



# Efficiency gain by pulsed nature

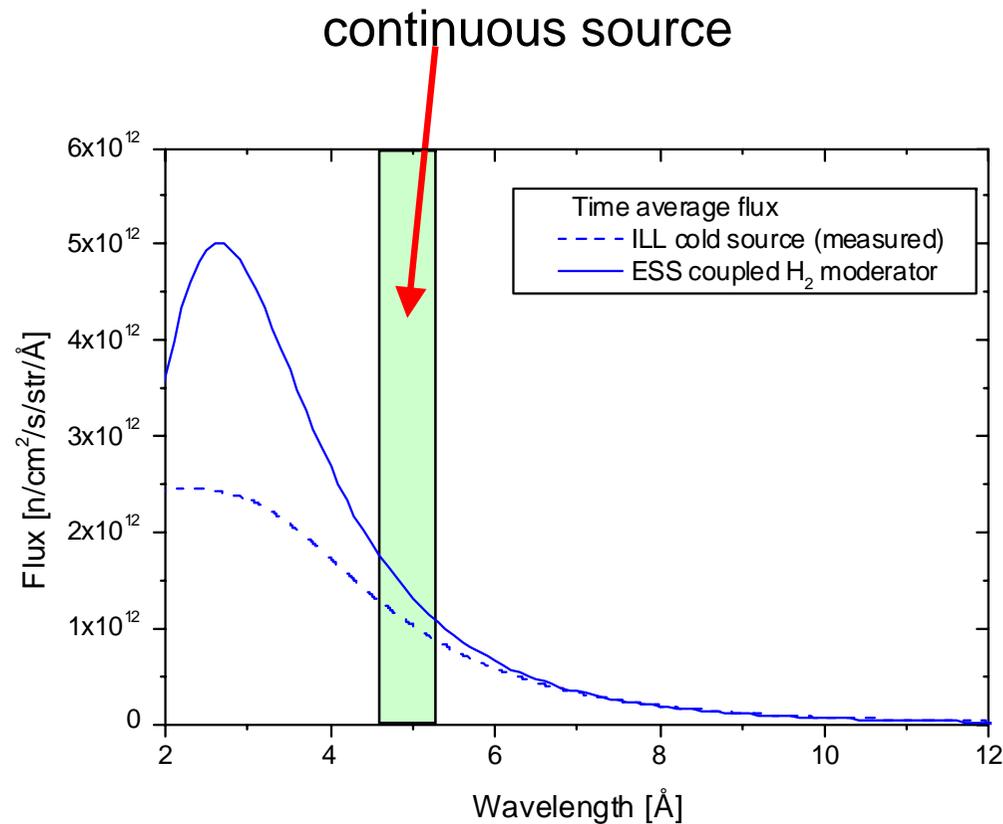
Part of spectrum used by a diffractometer for large structures (e.g. biological membranes)

continuous source



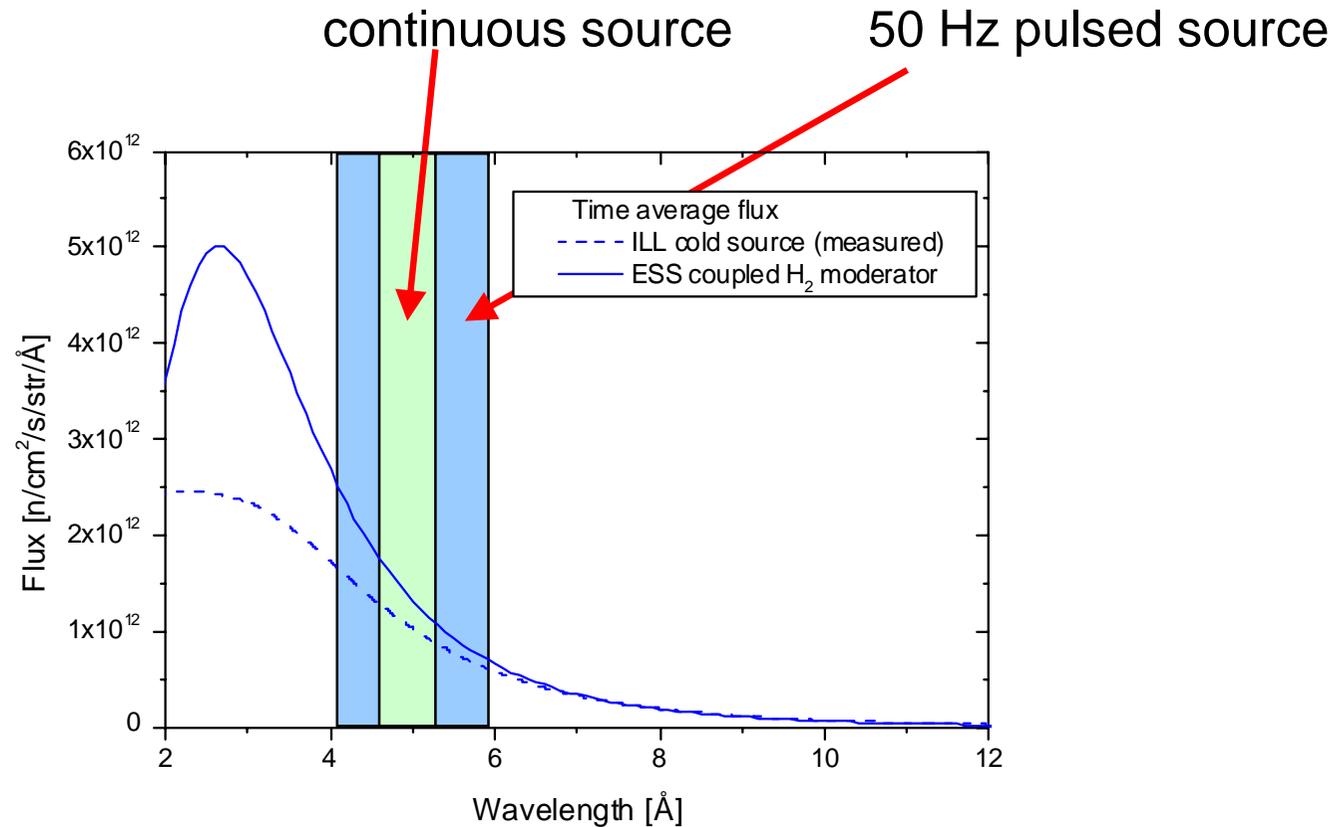
# Efficiency gain by pulsed nature

Part of spectrum used by a D22 (ILL) class instrument (Small Angle Neutron Scattering)



# Efficiency gain by pulsed nature

Part of spectrum used by a SANS instrument



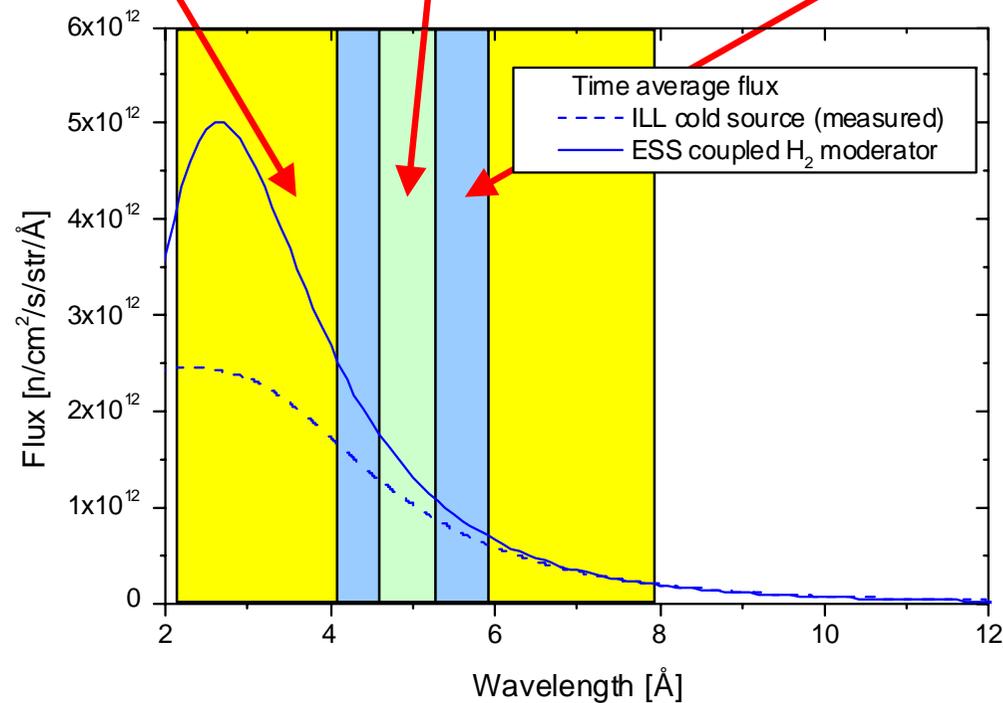
# Efficiency gain by pulsed nature

Part of spectrum used by a D22 (ILL) class instrument

16.67 Hz pulsed source

continuous source

50 Hz pulsed source



# Efficiency gain by pulsed nature

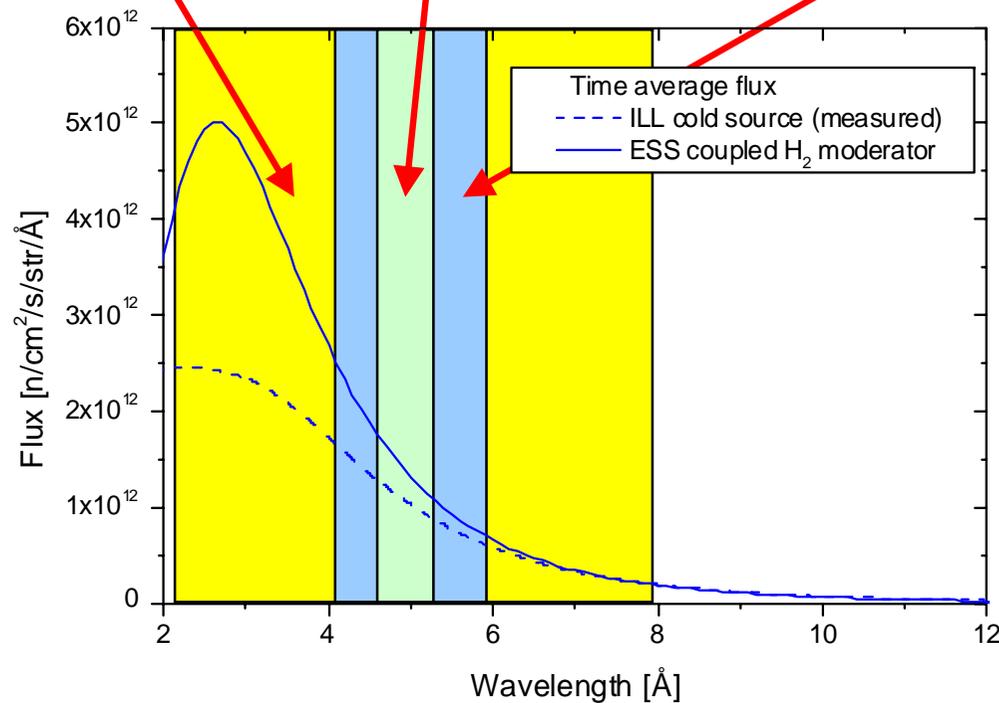
Part of spectrum used by a D22 (ILL) class instrument

16.67 Hz pulsed source

continuous source

50 Hz pulsed source

Efficiency gain  
by pulsing:  
 $\approx \delta\lambda/\lambda \sim 8-100$



# Efficiency gain by pulsed nature

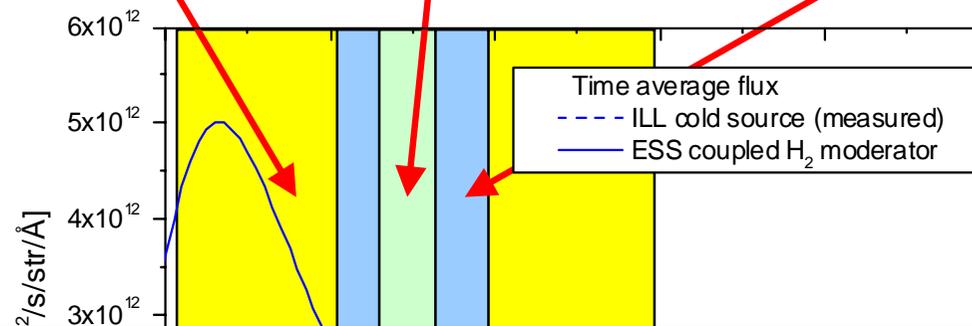
Part of spectrum used by a D22 (ILL) class instrument

16.67 Hz pulsed source

continuous source

50 Hz pulsed source

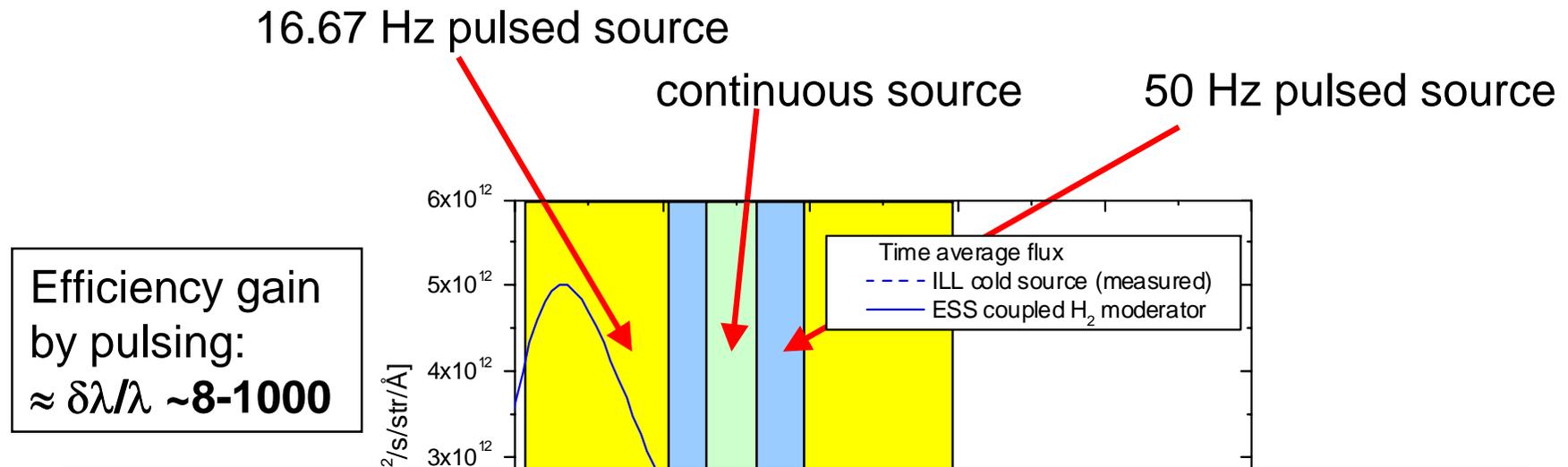
Efficiency gain  
by pulsing:  
 $\approx \delta\lambda/\lambda \sim 8-1000$



**Substantial overall progress beyond continuous sources in cold neutron research (soft matter, nanoscience): need to surpass their time average flux in low repetition rate**

# Efficiency gain by pulsed nature

Part of spectrum used by a D22 (ILL) class instrument



**Substantial overall progress beyond continuous sources in cold neutron research (soft matter, nanoscience): need to **surpass their time average flux in low repetition rate****  
**→ Large energy per pulse > 300 kJ**

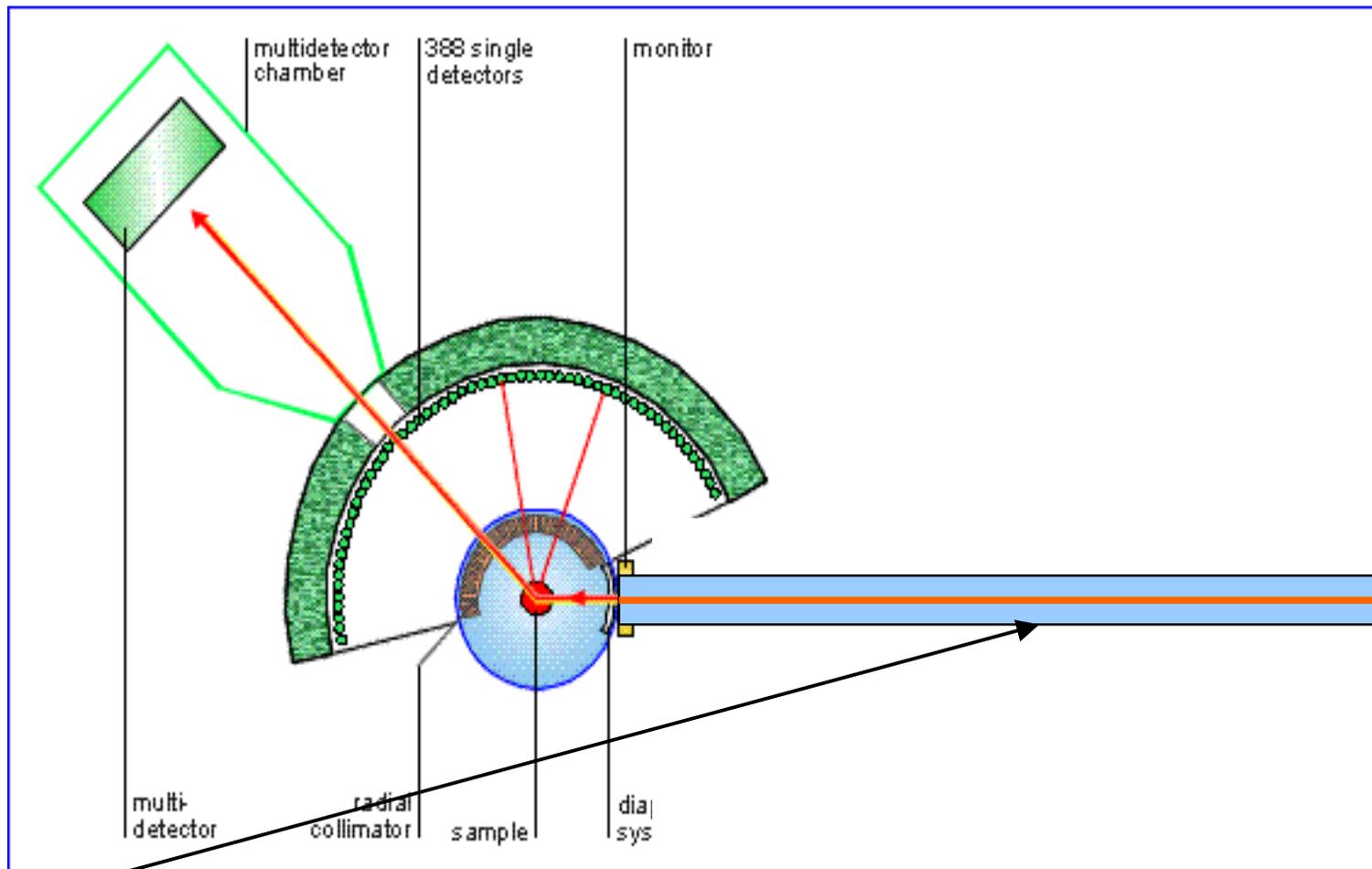
# Contradictory requirements by instruments

---

## Pulse parameters:

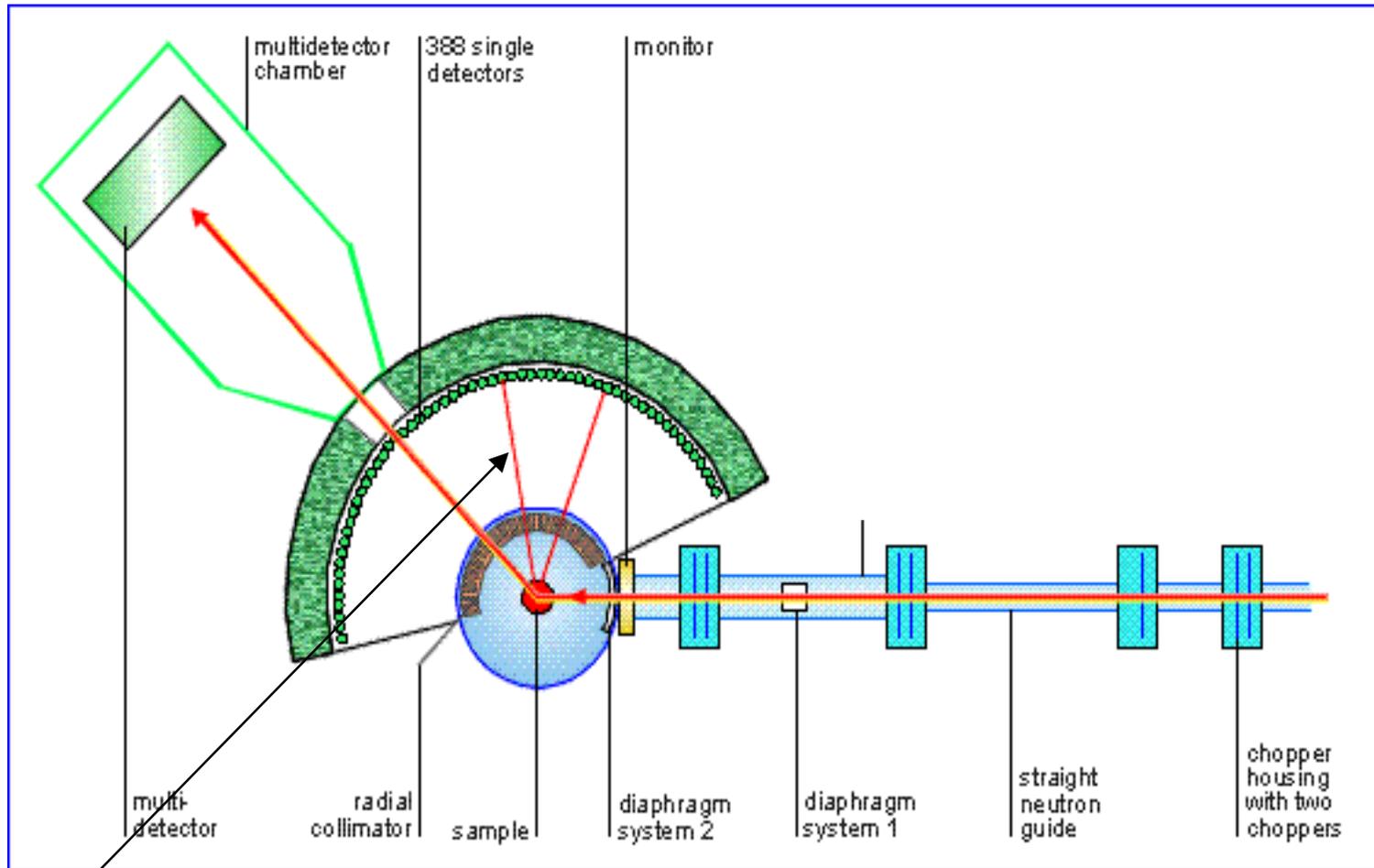
- **Duty factor  $c \sim$  resolution  $\delta\lambda/\lambda$**   
→ **low resolution vs. high resolution (0.1 % - 10 %)**
- **Pulse repetition rates  $\sim$  match neutron flight times**  
→ **(very) cold neutrons vs thermal/hot neutrons**  
    **elastic scattering: 5 vs. 100 Hz**  
    **inelastic scattering: 30 vs. 1000 Hz**

# Contradictory requirements by instruments



Flight path to determine repetition rate: 30-100 m for time-of-flight diffractometer

# Contradictory requirements by instruments



V3

Flight path to determine repetition rate: ~ 3 m for time-of-flight spectrometer

# Continuous vs. pulsed beams

---

## Ways to make neutrons monochromatic

- Time-of-flight: velocity  $v$

$$mv = h / \lambda$$

- Crystals: wavelength  $\lambda$

$$\lambda = 2d_{hkl} \sin\theta$$

$$v[\text{m/s}] = 3956 / \lambda[\text{\AA}]$$

# Continuous vs. pulsed beams

## Ways to make neutrons monochromatic

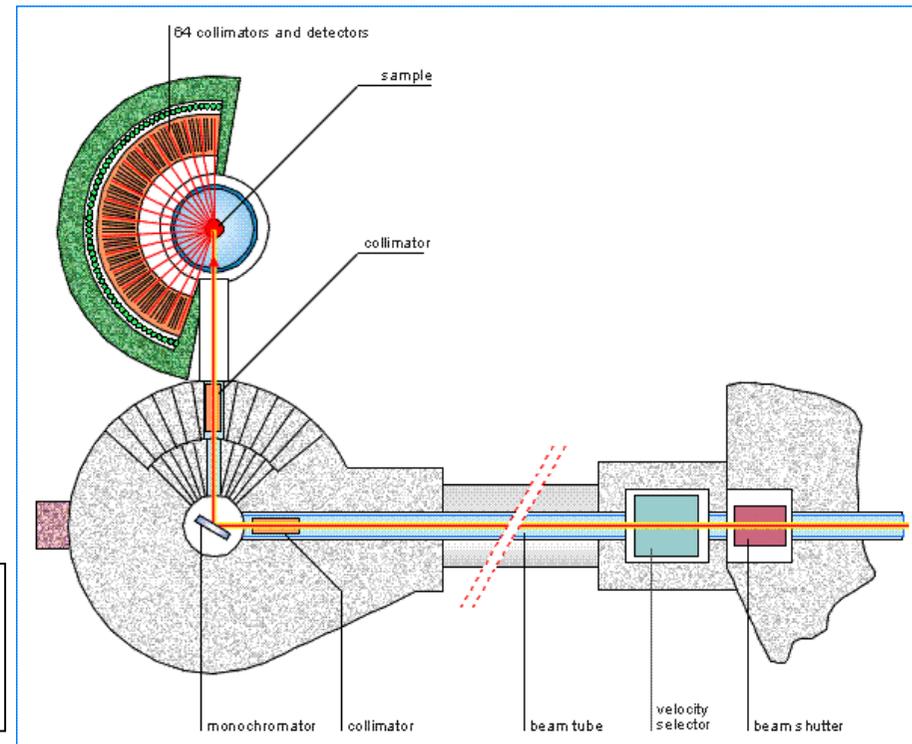
- Time-of-flight: velocity  $v$

$$mv = h / \lambda$$

- Crystals: wavelength  $\lambda$

$$\lambda = 2d_{hkl} \sin\theta$$

Powder Diffractometer  
(Continuous source)



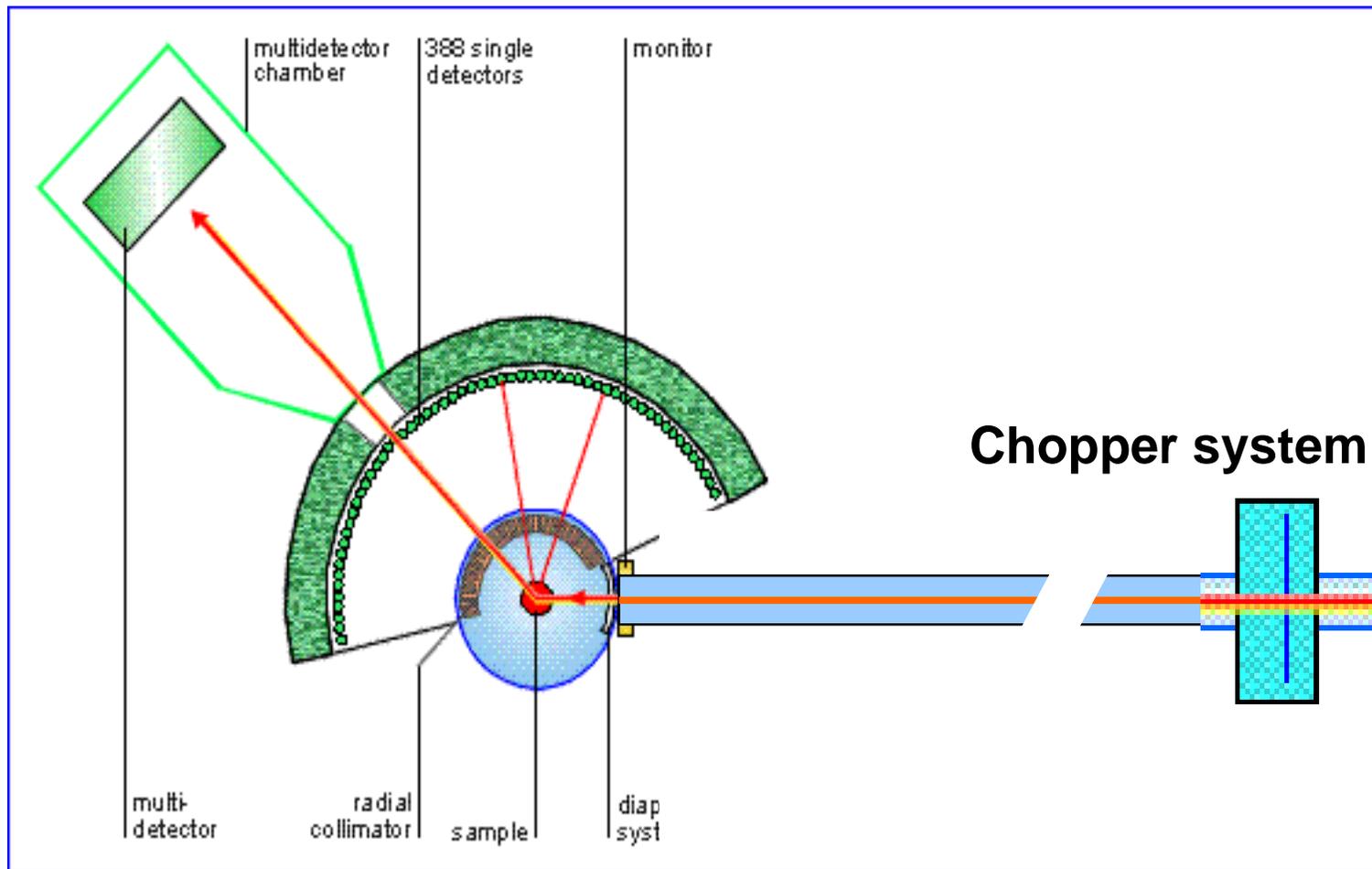
# Continuous vs. pulsed beams: Mean flux theorem

---

**On a continuous neutron source:**

**The time average (mean) neutron flux at the sample at equal wavelength and angular resolution is the same for both time-of-flight (TOF) and wavelength selection (crystal) monochromatization for reasonable TOF pulse repetition rate**

# TOF monochromatization at continuous source



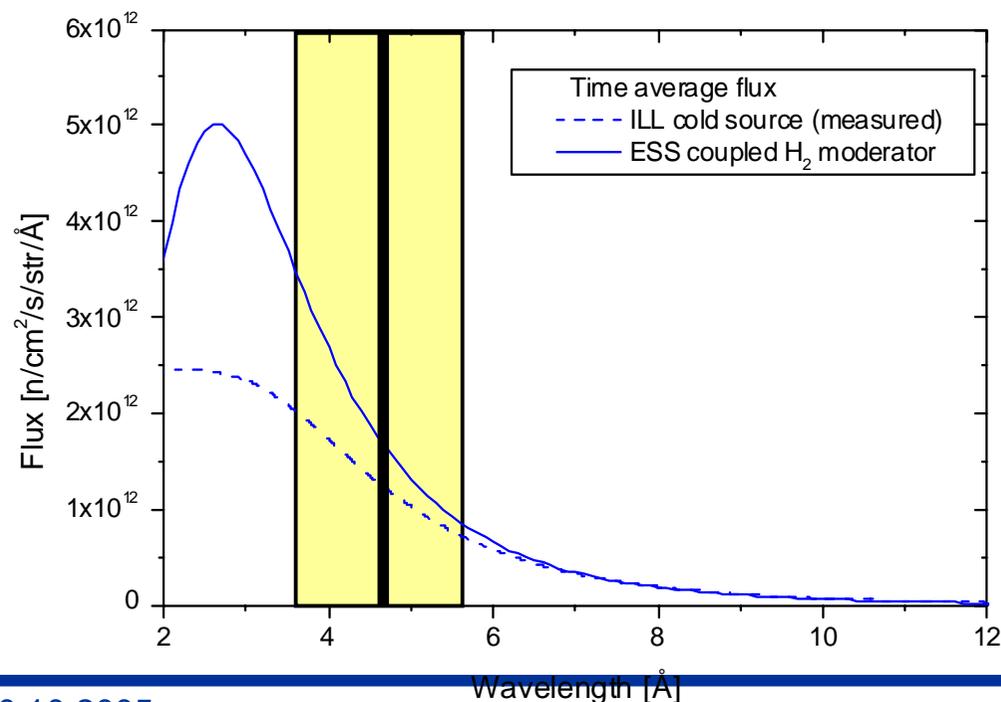
V3

Flight path to determine repetition rate: 30-100 m for time-of-flight diffractometer

# Continuous vs. pulsed beams: Mean flux theorem

On a continuous neutron source:

The time average (mean) neutron flux at the sample at equal wavelength and angular resolution **is the same for both time-of-flight (TOF) and wavelength selection (crystal) monochromatization for reasonable TOF pulse repetition rate**



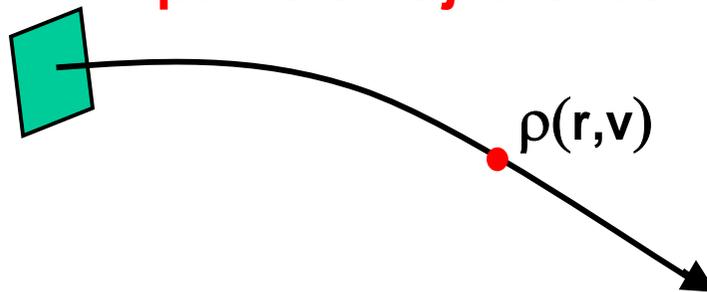
“narrow band”

Exercise!

# Continuous vs. pulsed beams: Mean flux theorem

Flux is governed by **Liouville theorem**:

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



*Absolute flux determination:*  
at any point along the beam

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

(absorption) loss factor  $\leq 1$

No. of particles hitting in unit time a surface perpendicular to trajectory (local z axis):

$$N = dx dy dz dv_x dv_y dv_z =$$

$$= \rho dx dy v v \alpha_x v \alpha_y v^2 d\lambda m/h \propto$$

$$\propto \phi(\lambda) df d\Omega d\lambda$$

where the brightness

$\phi(\lambda) = \rho mv^5/h$  **is a constant** if the neutron velocity is preserved (i.e. little acceleration)

Note: for Maxwellian tail  $\rho$  is independent of  $v$ .

# Continuous vs. pulsed beams: Mean flux theorem

---

**On a continuous neutron source:**

The time average (mean) neutron flux at the sample at equal wavelength and angular resolution **is the same for both time-of-flight (TOF) and wavelength selection (crystal) monochromatization for reasonable TOF pulse repetition rate**

**The brightness of the continuous source only matters, the pulsed (TOF) and continuous methods of beam monochromatization are equivalent!**

# Peak flux theorem

---

In neutron scattering work for a neutron source **with sufficiently long source pulses the peak flux alone matters**, independently of any reasonable source time structure (continuous or pulsed)

# Peak flux theorem

---

For an arbitrary source repetition rate  $f$  one will choose the instrument length  $L$  so that to assure the desired band  $\Delta\lambda$ :

$$L = A \Delta\lambda^{-1} f^{-1}$$

( $A=3956 \text{ \AA m/s}$ ). With this  $L$  the pulse length  $t$  for the required resolution  $\delta\lambda$  has to be

$$t = A^{-1} L \delta\lambda = f^{-1} (\delta\lambda / \Delta\lambda)$$

Can be as much as 10 % of  $f^{-1}=T$

The neutron flux on the sample will be given in terms of the peak source brightness function  $\Phi_p(\lambda)$ , beam divergence  $\delta\Omega$  and the efficiency factor of the beam delivery system  $\eta$

$$\varphi = \eta \delta\Omega t f \int \Phi_p(\lambda) d\lambda = \eta \delta\Omega (\delta\lambda / \Delta\lambda) \int \Phi_p(\lambda) d\lambda ,$$

Independent of  $f$

The integral is over the wavelength band  $\Delta\lambda = \lambda_{\max} - \lambda_{\min}$ .

# Peak flux theorem

---

What is “sufficiently long pulse  $t_{\min}$ ”?

- Irradiation work:  $\infty$
- Single  $(Q, \omega)$  experiments (D3, TAS?):  $\infty$
- SANS, NSE: 2 – 4 ms
- Reflectometry: 0.5 – 2 ms
- Single Xtal diffraction: 100 – 500  $\mu\text{s}$
- Powder diffraction: 5 – 500  $\mu\text{s}$
- Cold neutron spectroscopy: 50 – 2000  $\mu\text{s}$
- Thermal neutron spectroscopy: 20 – 600  $\mu\text{s}$
- Hot neutron spectroscopy: 10 – 300  $\mu\text{s}$
- Electronvolt spectroscopy: 1 – 10  $\mu\text{s}$
- Backscattering spectroscopy: 10 – 100  $\mu\text{s}$ , ...

**Rough estimate:**  $t_{\min} / T \sim \delta\lambda / \lambda$

# Peak flux theorem

---

## **Technical preconditions, enabling technologies:**

**Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ),**

# Peak flux theorem

---

## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ),

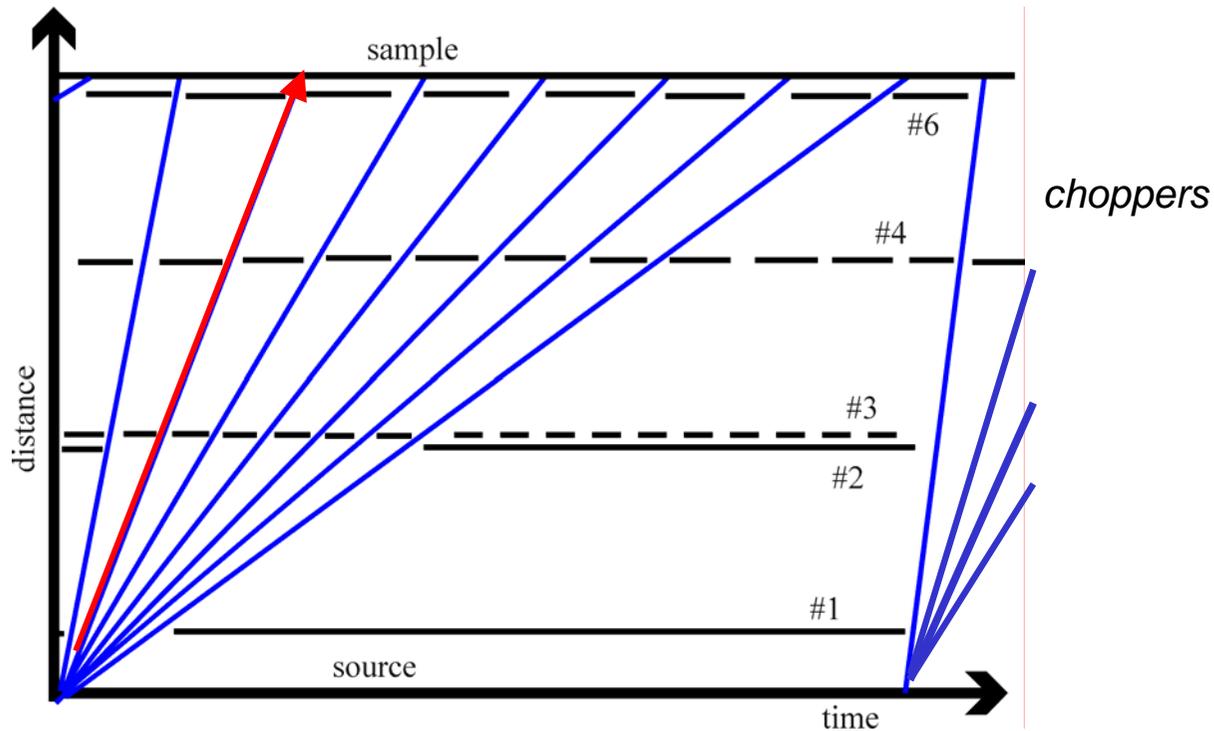
Repetition Rate Multiplication for TOF Spectroscopy: **to allow “reasonable” repetition rates both in diffraction (elastic scattering) and TOF spectroscopy (inelastic scattering) at the same time**

# Peak flux theorem

## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ),

Repetition Rate Multiplication for TOF Spectroscopy: **to allow “reasonable” repetition rates both in diffraction (elastic scattering) and TOF spectroscopy (inelastic scattering) at the same time**



# Peak flux theorem

---

## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ )

Repetition Rate Multiplication for TOF Spectroscopy

Pulse shaping: **to allow to choose the best pulse length for each application**

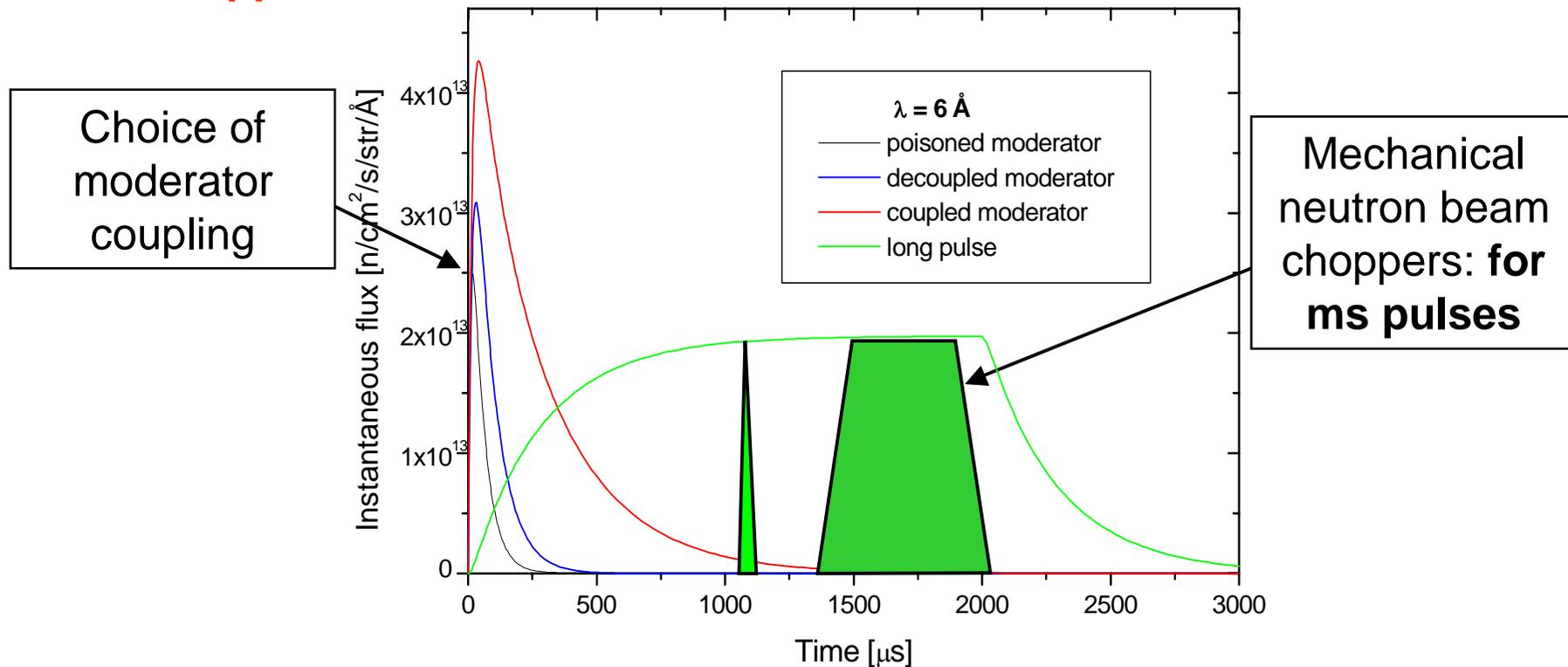
# Peak flux theorem

## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ),

Repetition Rate Multiplication for TOF Spectroscopy

Pulse shaping: **to allow to choose the best pulse length for each application**



# Peak flux theorem

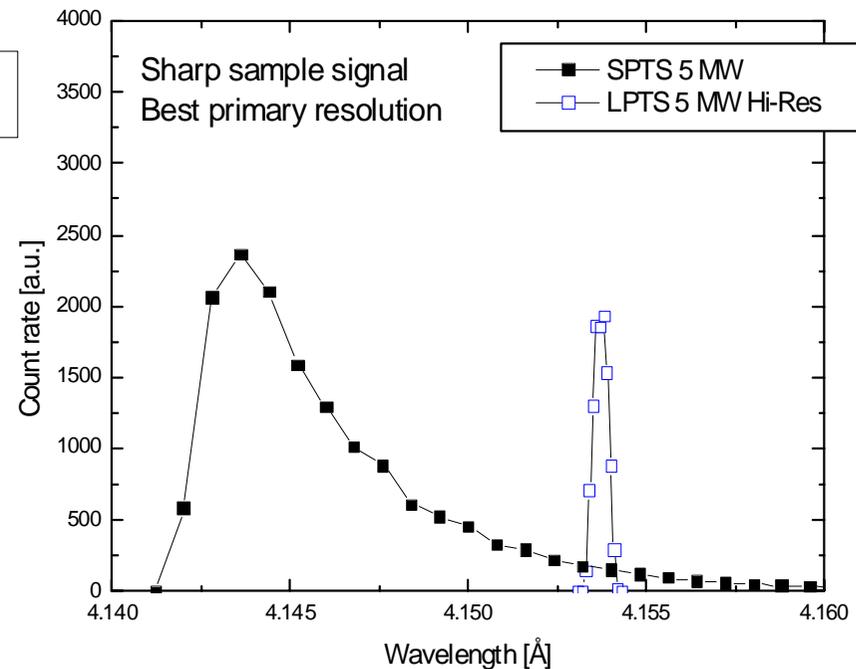
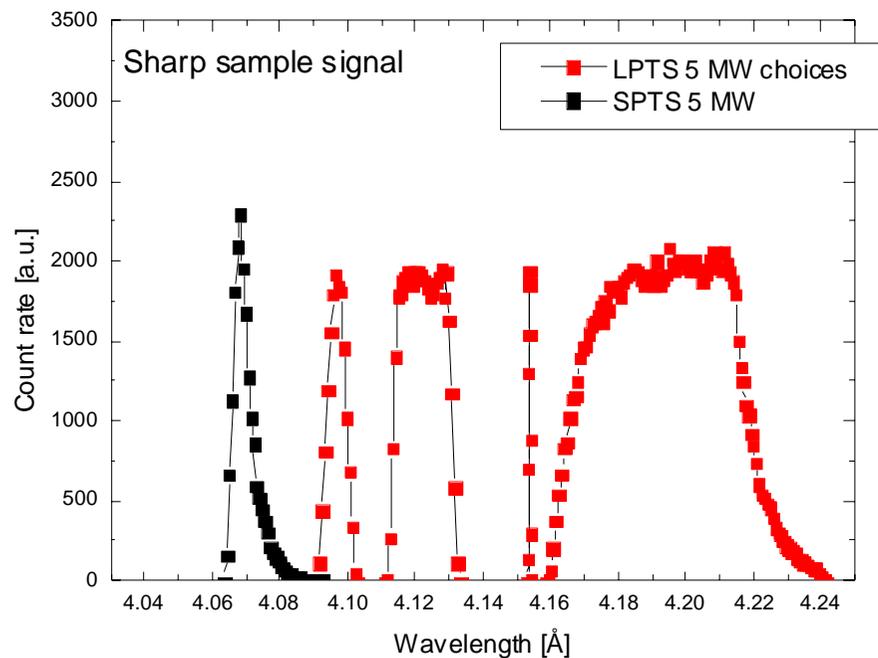
## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ),

Repetition Rate Multiplication for TOF Spectroscopy

**Pulse shaping: to allow to choose the best pulse length in each experiment on the same instrument**

E.g. variable resolution powder diffraction: trade intensity  $\leftrightarrow$  resolution



# Peak flux theorem: resolution of contradictory needs

---

## Technical preconditions, enabling technologies:

Advanced neutron guides (low loss at any L for  $\lambda > 1 \text{ \AA}$ ): **to make the distance L a free parameter**

Repetition Rate Multiplication for TOF Spectroscopy: **to allow “reasonable” repetition rates both in diffraction (elastic scattering) and TOF spectroscopy (inelastic scattering) at the same time**

Pulse shaping: **to allow to choose the best pulse length for each application**

**Engineering reality: guides and choppers work with full efficiency for thermal and cold neutrons only  
( $E < 100 \text{ meV}$ )**

# Peak flux theorem: optimization criteria

---

## Highest peak flux and longest pulses

**Ideal solutions are unrealistic:**

**CW source with infinite brightness**

**Pulsed source with infinite intensity**

# Accelerator / target realities vs. instruments

---

## Neutron moderation time

- lower limit on neutron pulse length  $\tau$
- peak flux:  $\propto E_p / \tau$
- decoupled moderators with shorter moderation time are of disproportionately lower efficiency

# Accelerator / target realities vs. instruments

---

## Neutron moderation time

- lower limit on neutron pulse length  $\tau$
- peak flux:  $\propto E_p / \tau$
- decoupled moderators with shorter moderation time are of disproportionately lower efficiency

## Proton beam energy per pulse $E_p$ technologically limited

- to  $< 50 - 100$  kJ (?) for  $\mu\text{s}$  short proton pulses (from rings):  $W_{\text{instant}} > 50 \text{ GW}$
- to  $< 500 - 2000$  kJ (?) for ms pulses (from linacs)  
 $W_{\text{instant}} > 0.5 \text{ GW}$

# Accelerator / target realities vs. instruments

---

## Neutron moderation time

- lower limit on neutron pulse length  $\tau$
- peak flux:  $\propto E_p / \tau$
- decoupled moderators with shorter moderation time are of disproportionately lower efficiency

## Proton beam energy per pulse $E_p$ technologically limited

- to  $< 50 - 100$  kJ (?) for  $\mu\text{s}$  short proton pulses (from rings):  $W_{\text{instant}} > 50 \text{ GW}$
- to  $< 500 - 2000$  kJ (?) for ms pulses (from linacs)  
 $W_{\text{instant}} > 0.5 \text{ GW}$

→ highest time average flux requires long pulses

# Accelerator / target realities vs. instruments

---

## Neutron moderation time

- lower limit on neutron pulse length  $\tau$
- peak flux:  $\propto E_p / \tau$
- decoupled moderators with shorter moderation time are of disproportionately lower efficiency

## Proton beam energy per pulse $E_p$ technologically limited

- to  $< 50 - 100$  kJ (?) for  $\mu\text{s}$  short proton pulses (from rings):  $W_{\text{instant}} > 50$  GW
- to  $< 500 - 2000$  kJ (?) for ms pulses (from linacs)  
 $W_{\text{instant}} > 0.5$  GW

→ highest time average flux requires long pulses

→ highest peak flux is achieved by long pulses for moderation times  $> 50 - 100 \mu\text{s}$  (thermal & cold neutrons)

# Long pulse approach

---

**Optimized spallation neutron source:**

**Maximum peak proton beam power in ms pulses**

**Possible (optimistic?) parameters for H<sup>+</sup> only linear accelerator:**

**3 GeV, 150 mA proton beam**

**2 ms pulses**

**20 Hz repetition rate → 18 MW beam power**

# Long pulse approach

---

**Optimized spallation neutron source:**

**Maximum peak proton beam power in ms pulses**

**Possible (optimistic?) parameters for H<sup>+</sup> only linear accelerator:**

**3 GeV, 150 mA proton beam**

**2 ms pulses**

**20 Hz repetition rate → 18 MW beam power**

**Compromise options to lower power:**

**shorter pulses: lower performance for low resolution, cold  
neutron work**

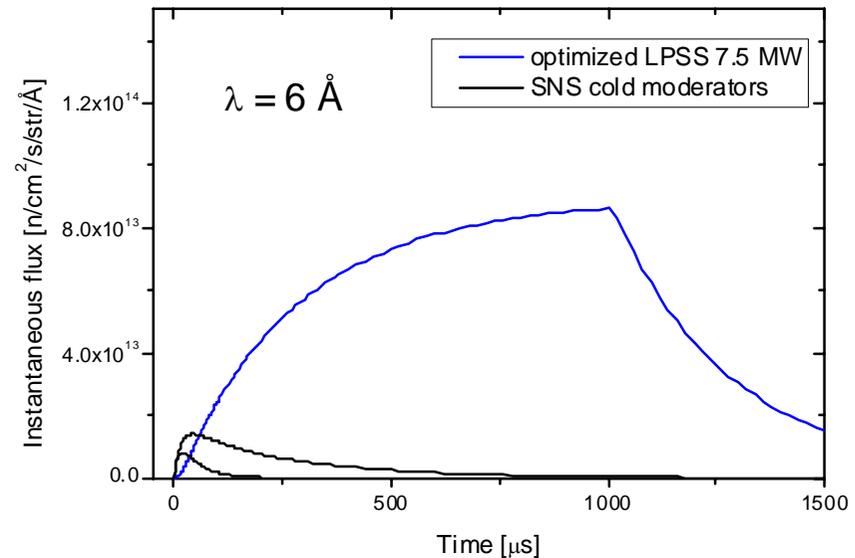
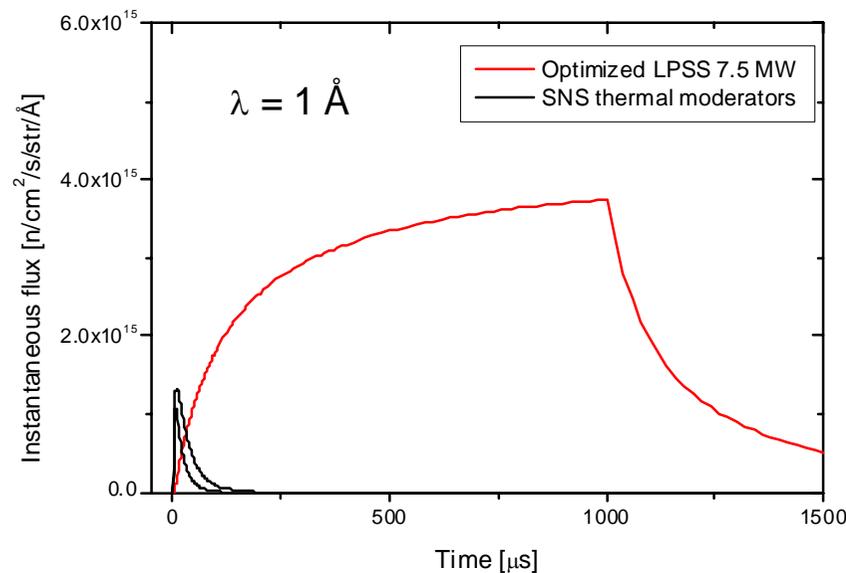
**lower repetition rate: lower thermal neutron performance**

**lower peak power: all applications affected**

# Long pulse approach

Optimized long pulse sources can produce not only **higher time average**, but also **higher peak flux** than short pulses in the cold and thermal neutron range (above 3 and 6 times higher energy/pulse, respectively).

Example: 450 kJ/pulse long pulses, vs 23 kJ/pulse short pulse (SNS at 1.4 MW):



**Long pulses: highest cold and thermal neutron peak flux at given costs**

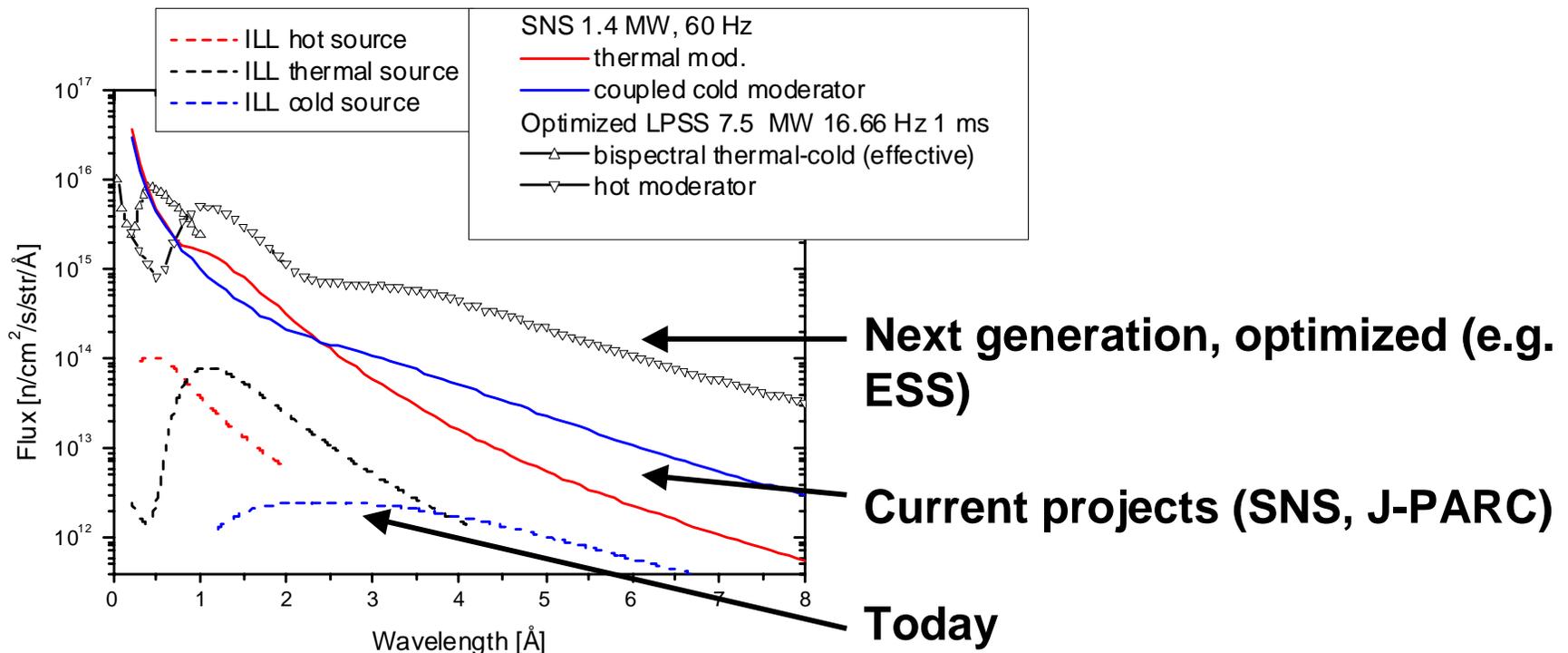
# Optimized approach

**Long pulses:** optimum for thermal and cold neutrons (~90 % of condensed matter research)

**Short pulses:** superior for  $\lambda < 0.4 - 0.9 \text{ \AA}$ .

**Long (enough) pulses:** performance scales with peak flux

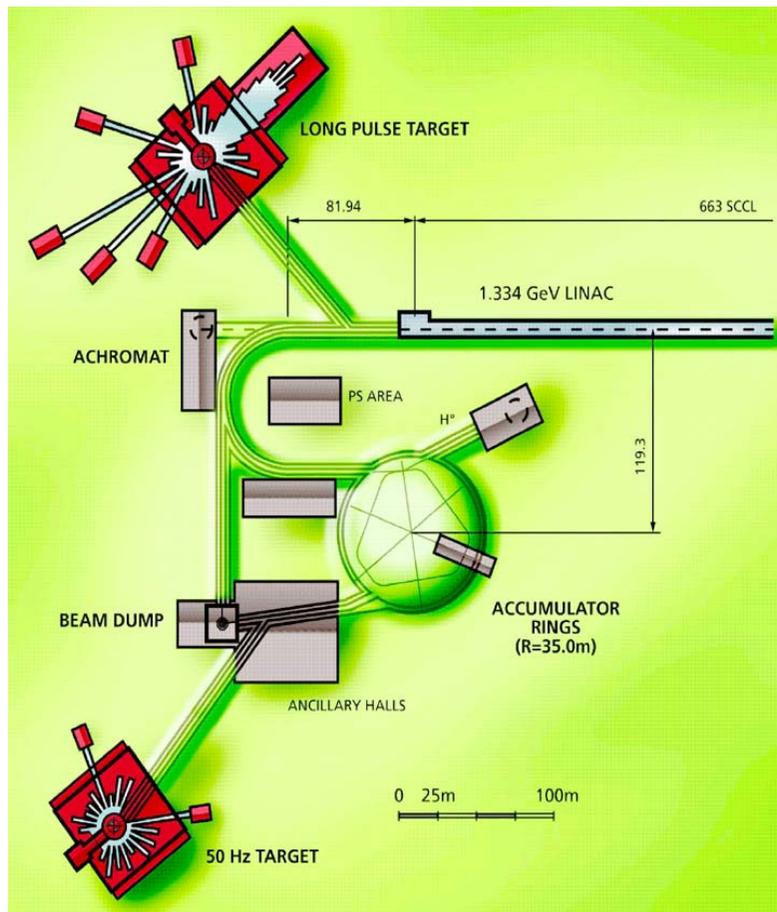
**Short pulses:** performance  $\leq$  peak flux



# Optimized approach

**Long pulses:** optimum for thermal and cold neutrons (~90 % of condensed matter research)

**Short pulses:** superior for  $\lambda < 0.4 - 0.9 \text{ \AA}$ .

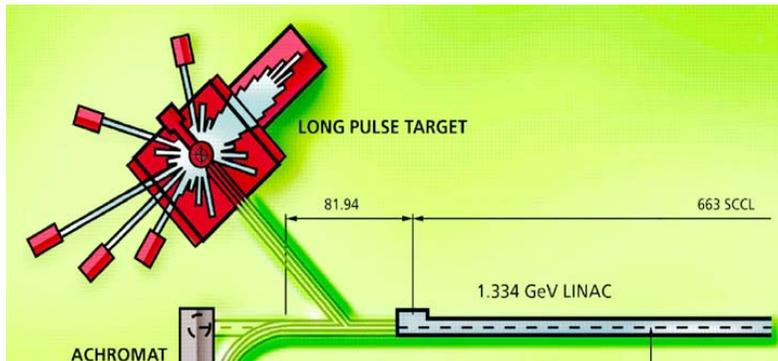


European Spallation Source project: combine both capabilities

# Optimized approach

**Long pulses:** optimum for thermal and cold neutrons (~90 % of condensed matter research)

**Short pulses:** superior for  $\lambda < 0.4 - 0.9 \text{ \AA}$ .



European Spallation Source staged realization plan:  
(Sweden, UK, Hungary,..??)

Long pulse only:

- much simpler technically
- easier to operate
- most cost effective

Later upgrade options:

- add short pulse station, *if there still worldwide need (SNS, J-PARC, ILL)*
- enhance long pulse power

# Conclusion

**Optimized spallation sources: orders of magnitude enhanced research opportunities in condensed matter research by neutron scattering.**

