Instrument Modelling Analytical Methods

6th April 2016

Ken Andersen

EUROPEAN SPALLATION SOURCE

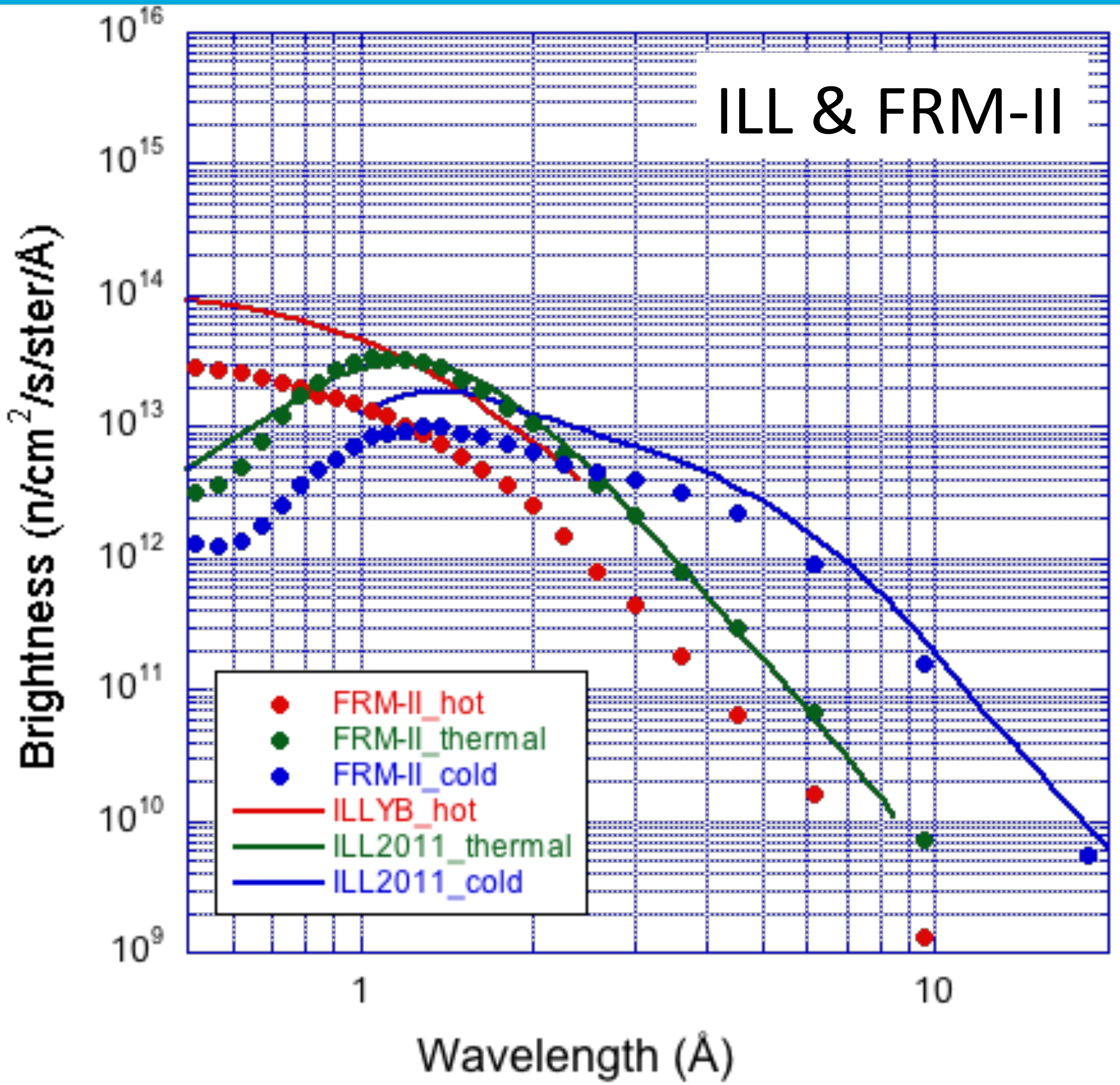
Slow Neutrons vs Light

	light	neutrons
λ	< μm	< nm
E	> eV	> meV
n	1→4	0.9997→1.0001
θ_c	90°	1°
B	10^{18} p/cm²/ster/s (60W lightbulb)	10^{14} n/cm²/ster/s (60MW reactor)
spin	1	½
interaction	electromagnetic	strong force, magnetic
charge	0	0

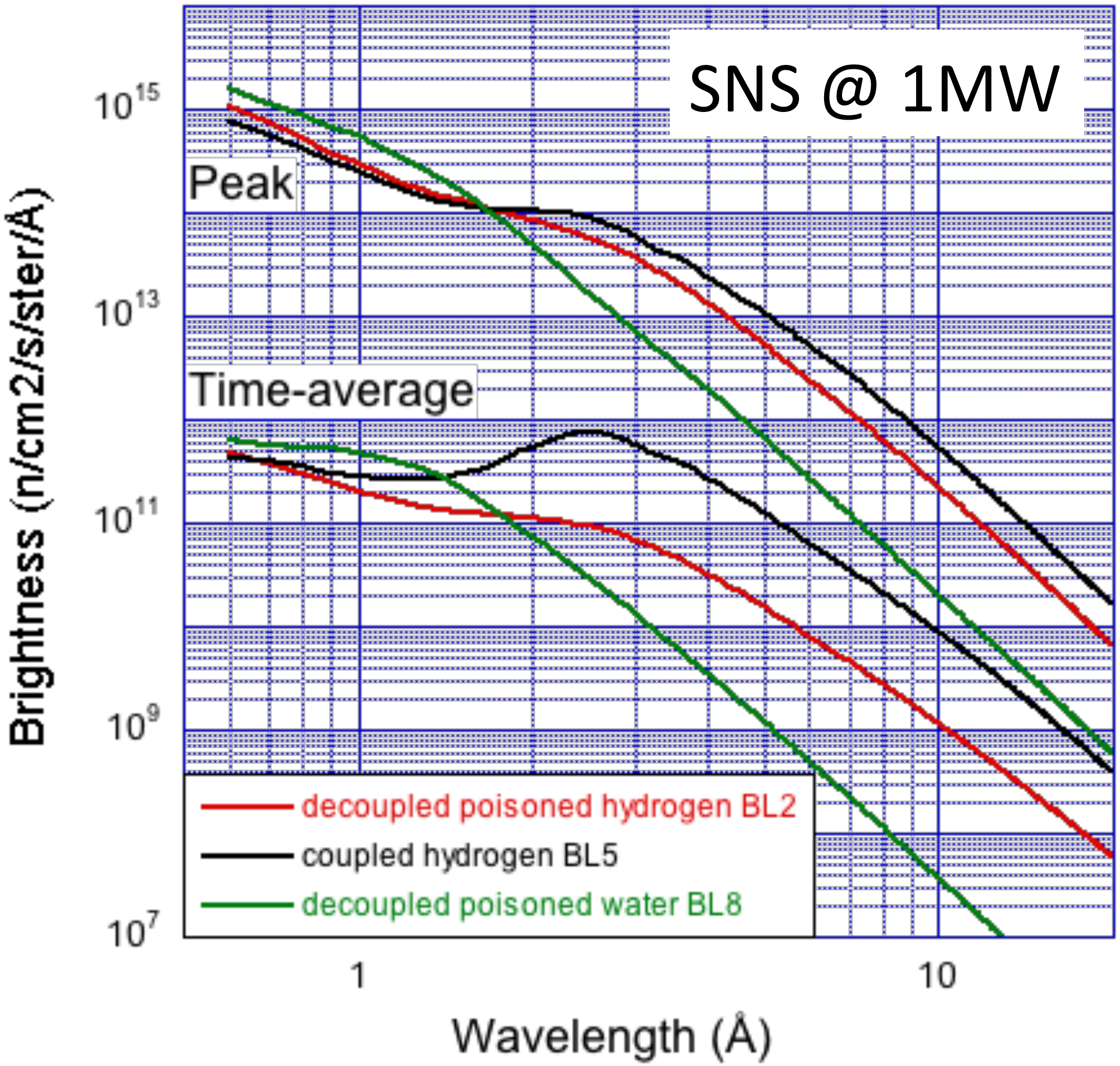
Topics

- Flux calculations
  - source brightness
  - brilliance transfer
  - calculation of flux given instrument parameters
  - example: ESS powder diffractometer
  - example: SNS STS chopper spectrometer
- Resolution calculations
  - calculation of instrument parameters given resolution requirement
  - formulate the measurement requirement
  - calculate partial differentials
  - match resolution contributions
  - example: ESS powder diffractometer
  - example: SNS STS chopper spectrometer

Source Brightness



Source Brightness



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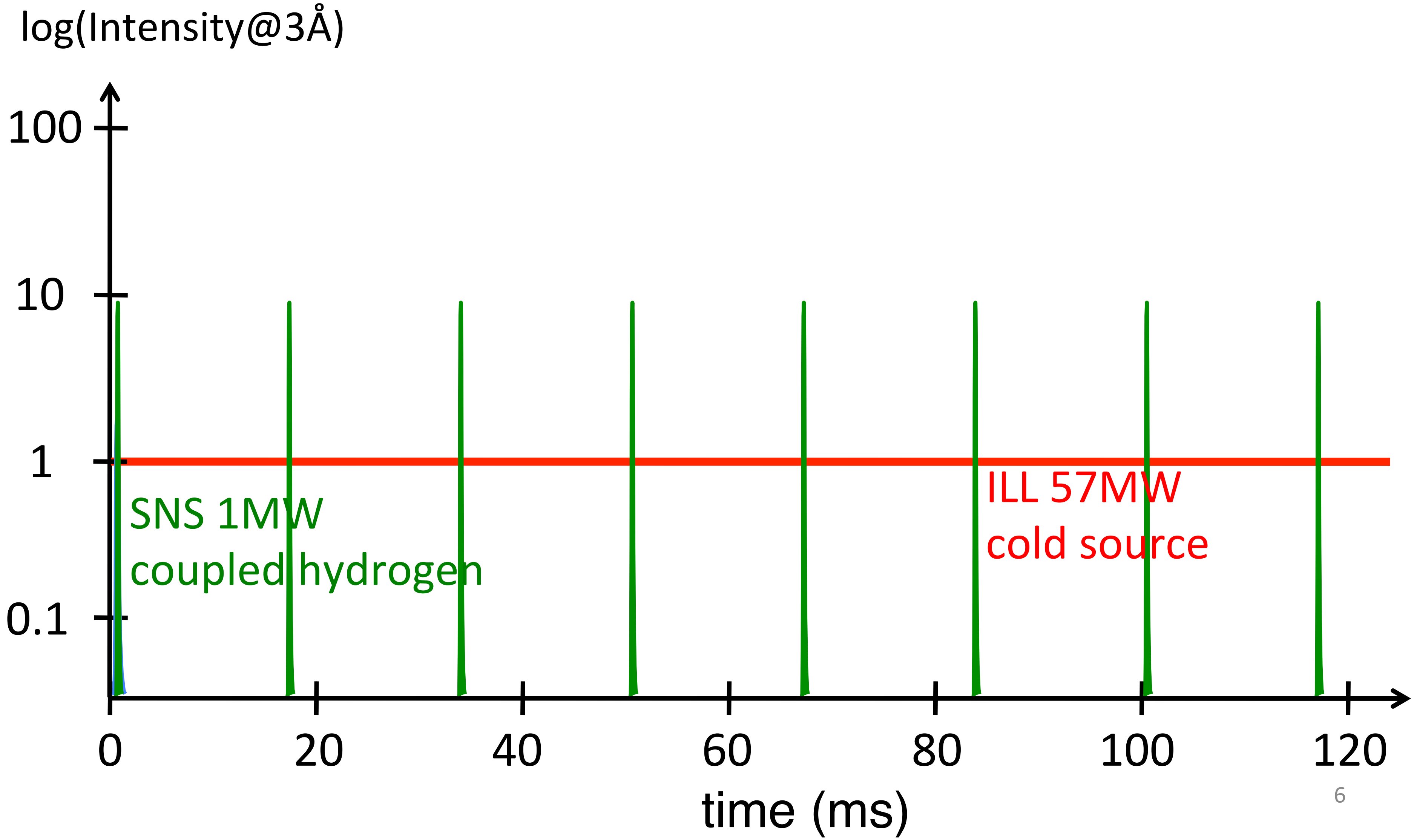

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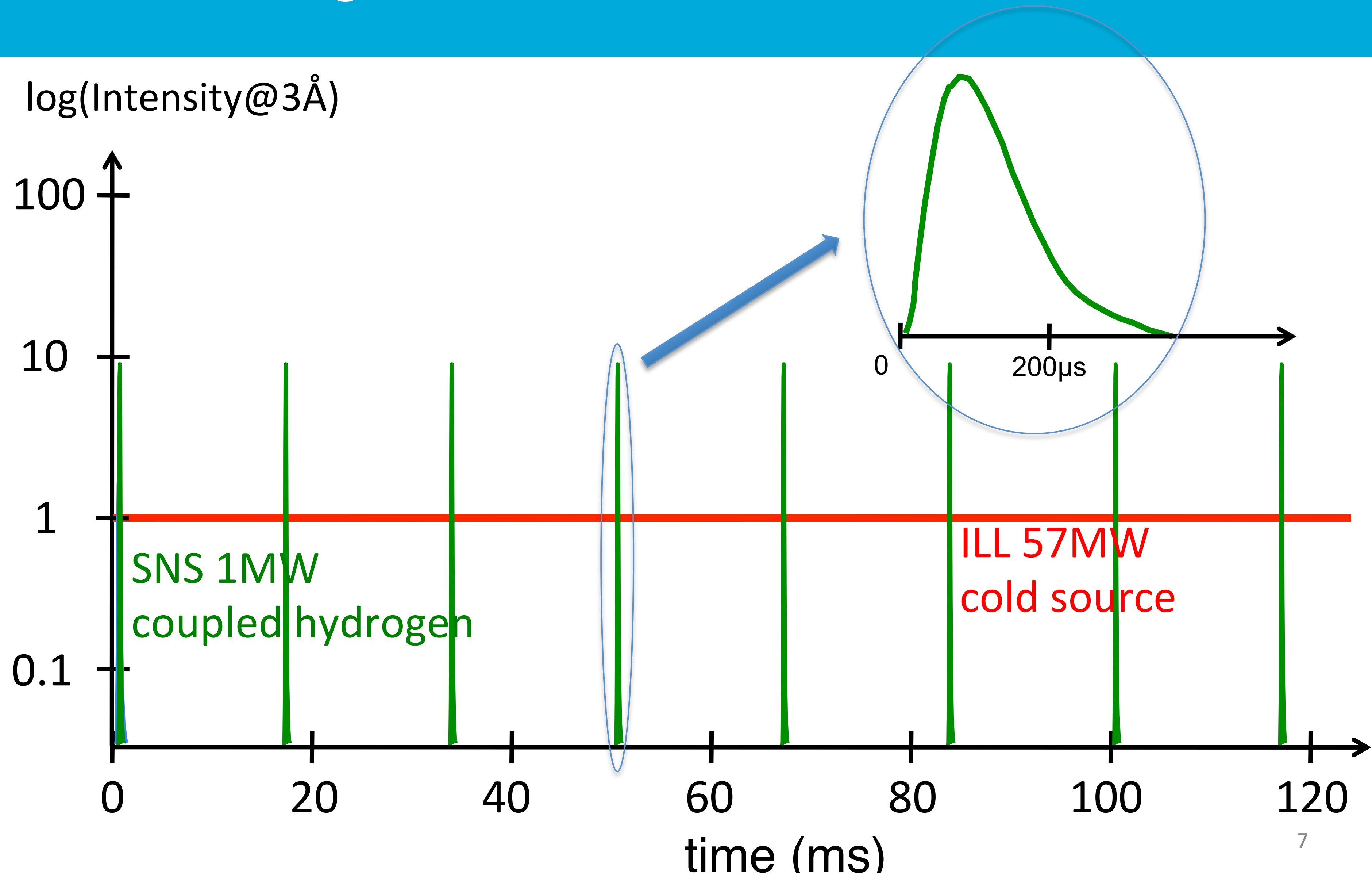

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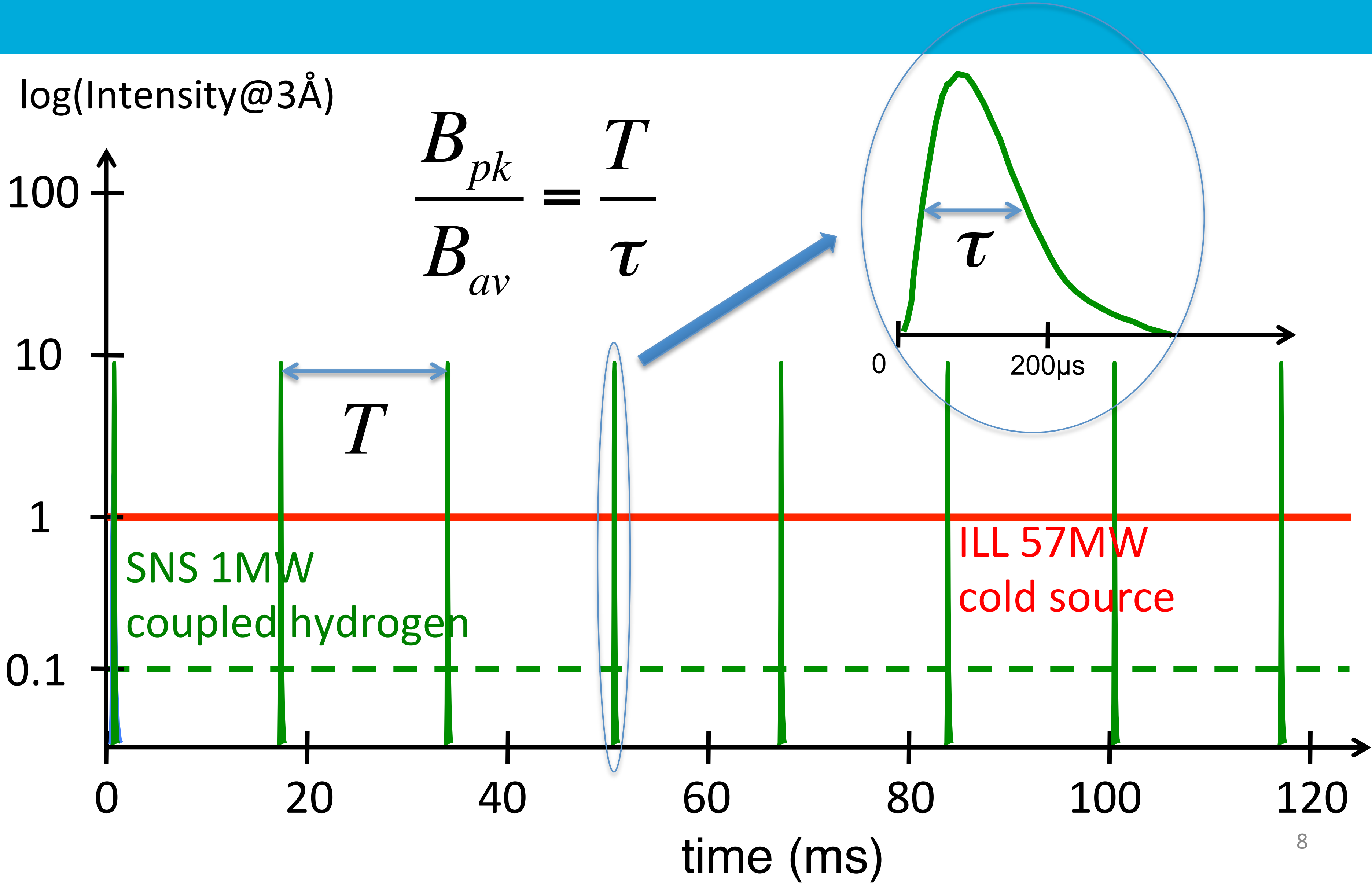

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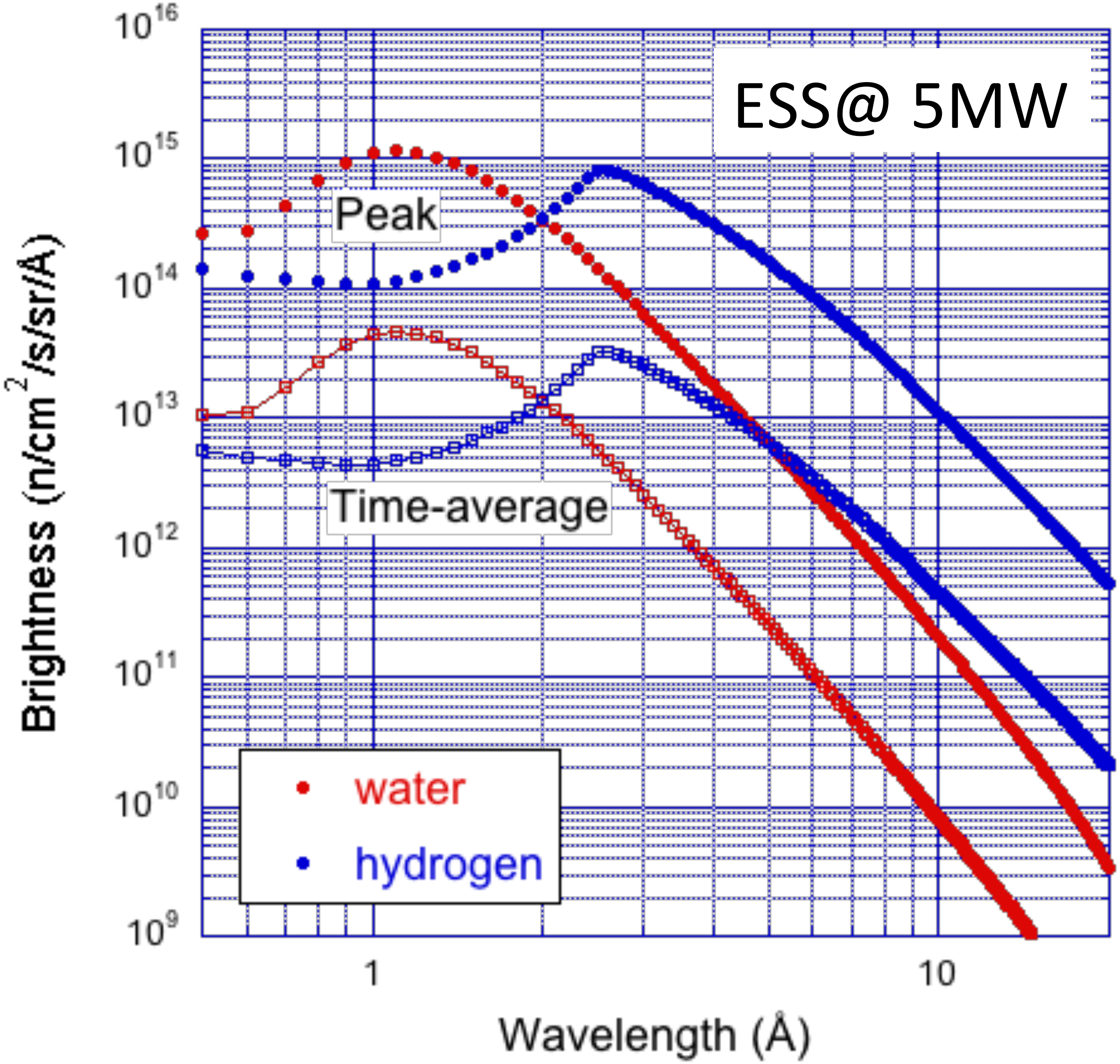

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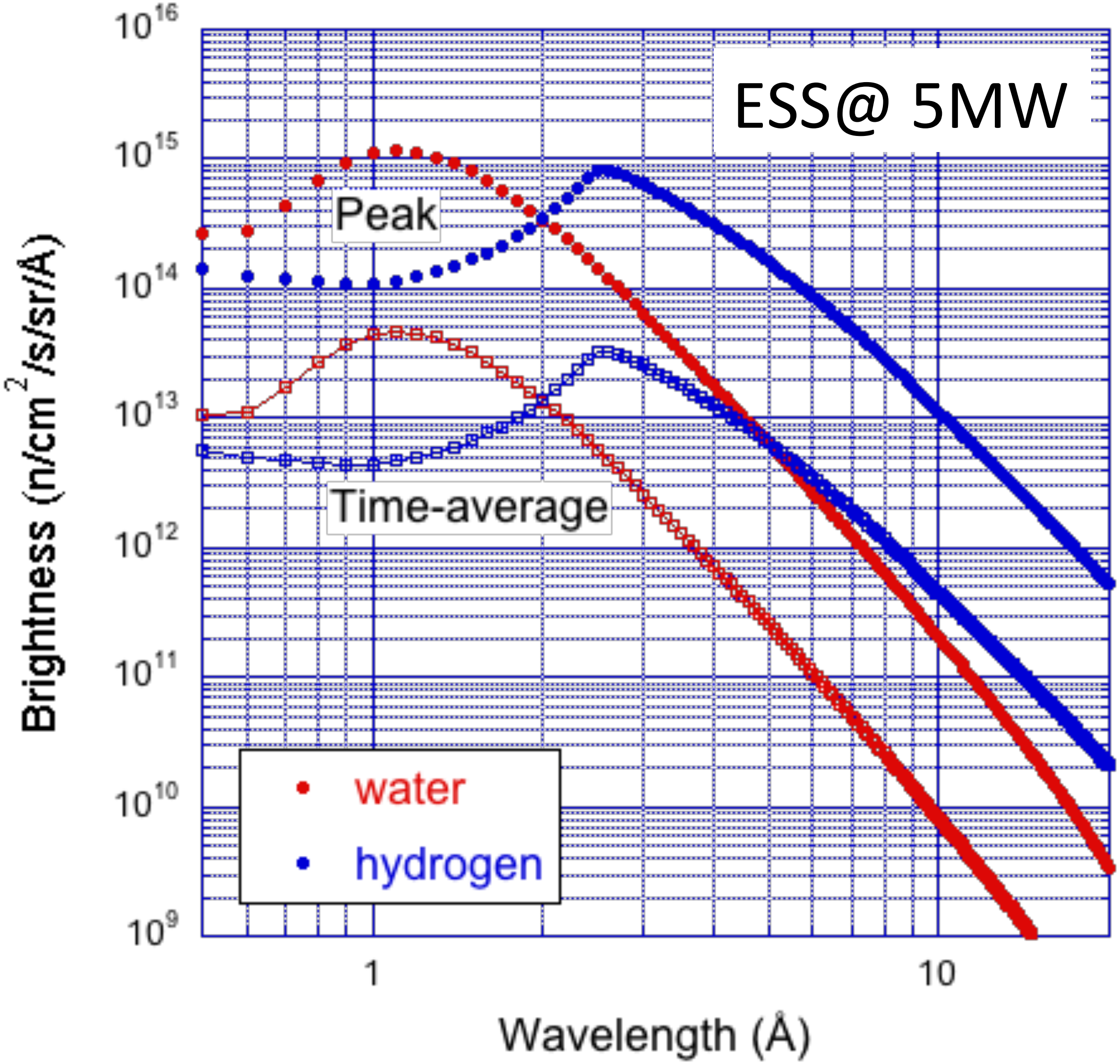
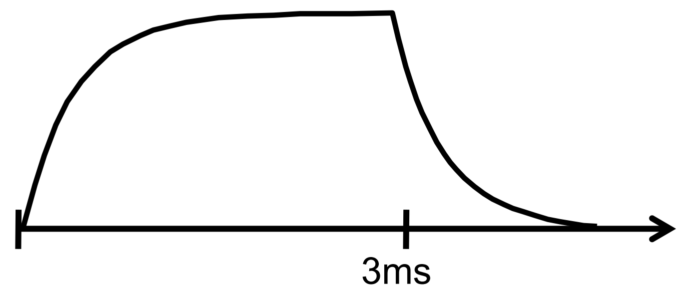




$$\frac{B_{pk}}{B_{av}} = \frac{T}{\tau} = 25$$

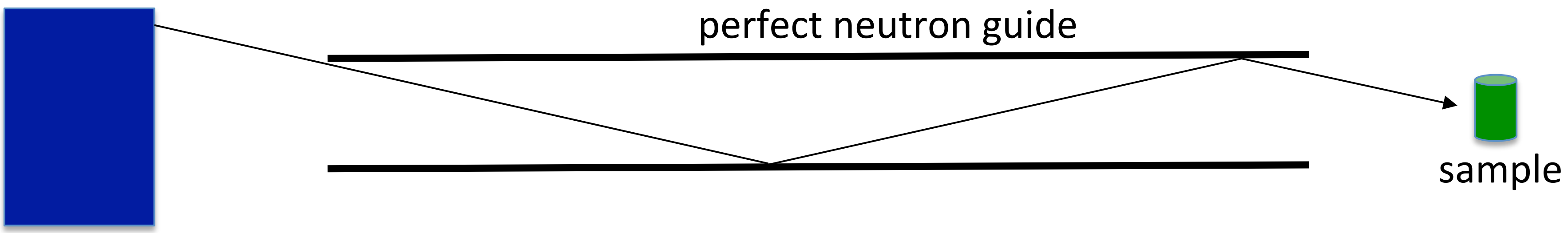
Flux Calculations

- Basic approach: $$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\, \mathrm{d}\lambda \times \Delta\Omega$$

Flux Calculations

- Basic approach: $$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\,\mathrm{d}\lambda \times \Delta\Omega$$
- Transported solid angle: $$\Delta\Omega = \Delta\theta_H \times \Delta\theta_V \times BT$$
- *BT* = Brilliance Transfer: between 0 and 1
  - how effective the guide system is
  - if you don't know, set it to 0.5

Guide Illumination



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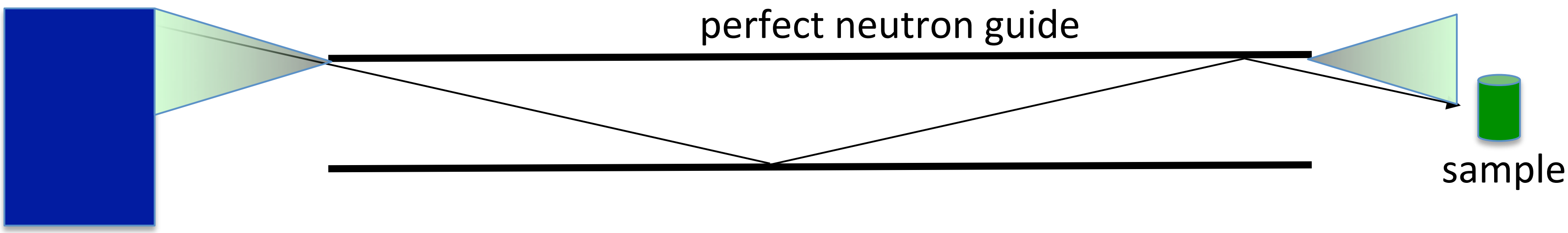
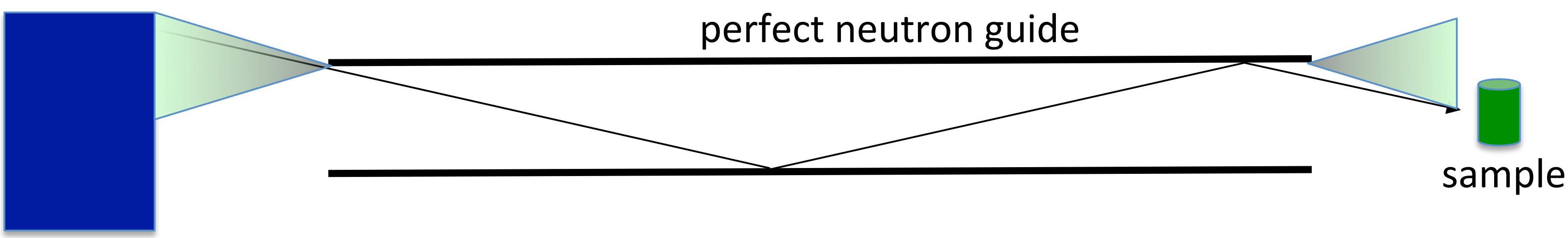


“over-illumination”

Beam requirements:

- Area
- Divergence range
- Wavelength range

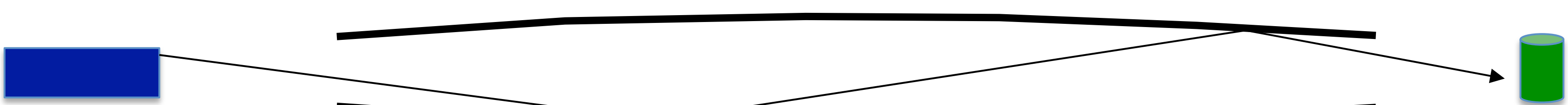
Guide Illumination



"over-illumination"

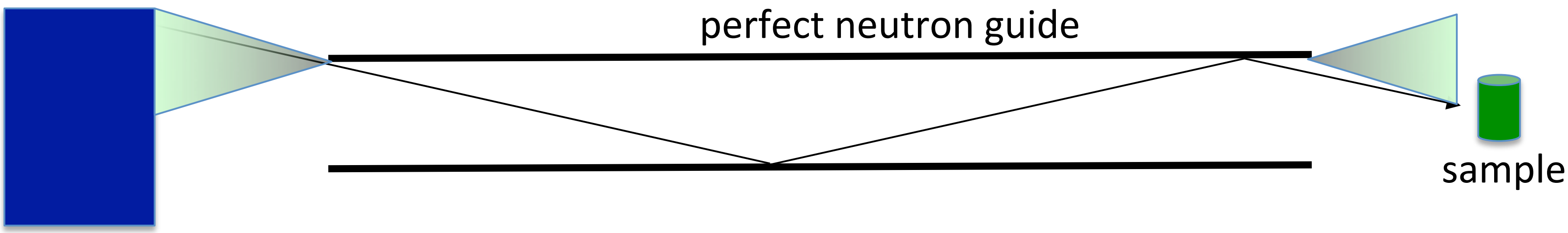
Perfect Brilliance Transfer

Beam requirements:
- Area
- Divergence range
- Wavelength range



"under-illumination"

Guide Illumination



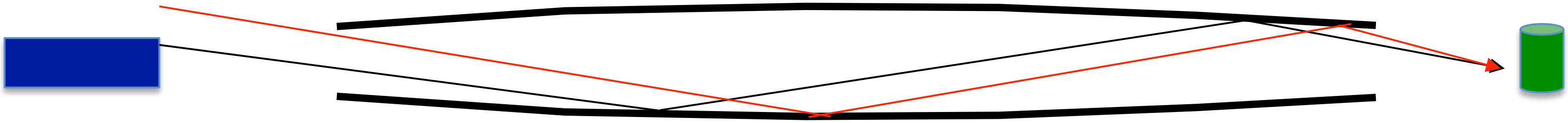
"over-illumination"

Perfect Brilliance Transfer

Beam requirements:

- Area
- Divergence range
- Wavelength range

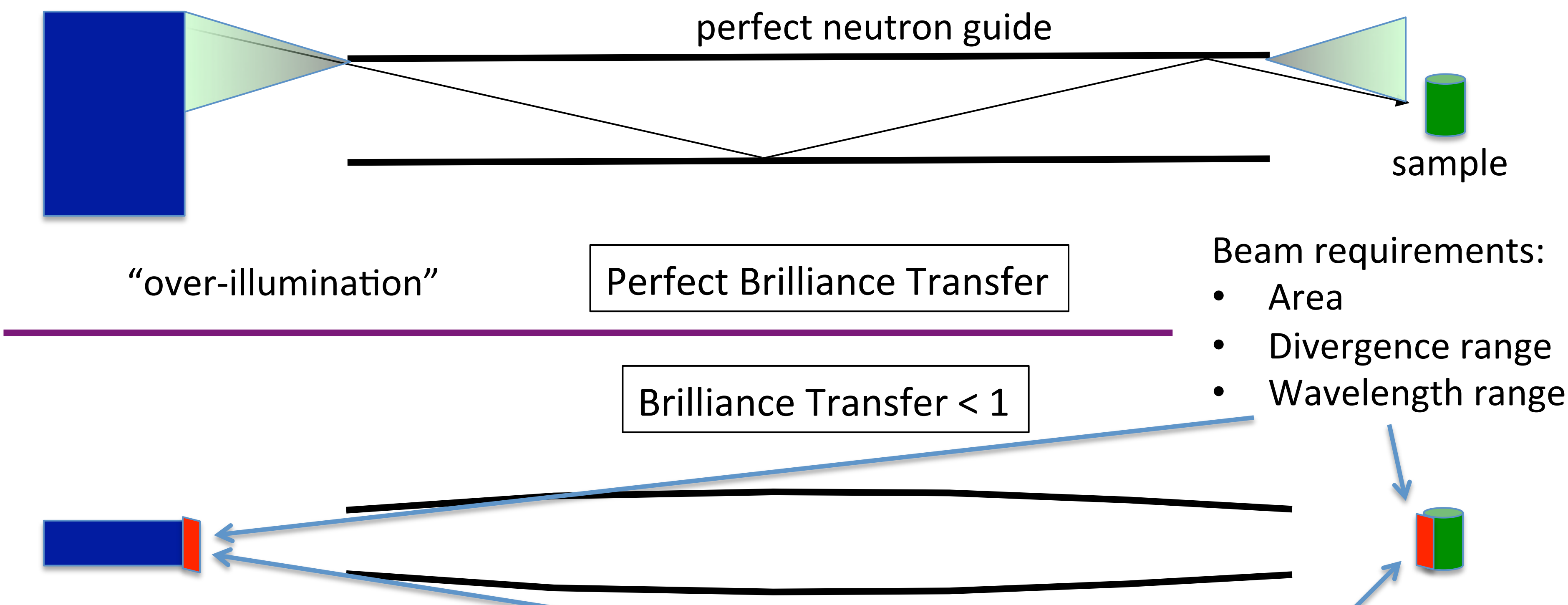
Brilliance Transfer < 1



"under-illumination"

=> less efficient guides

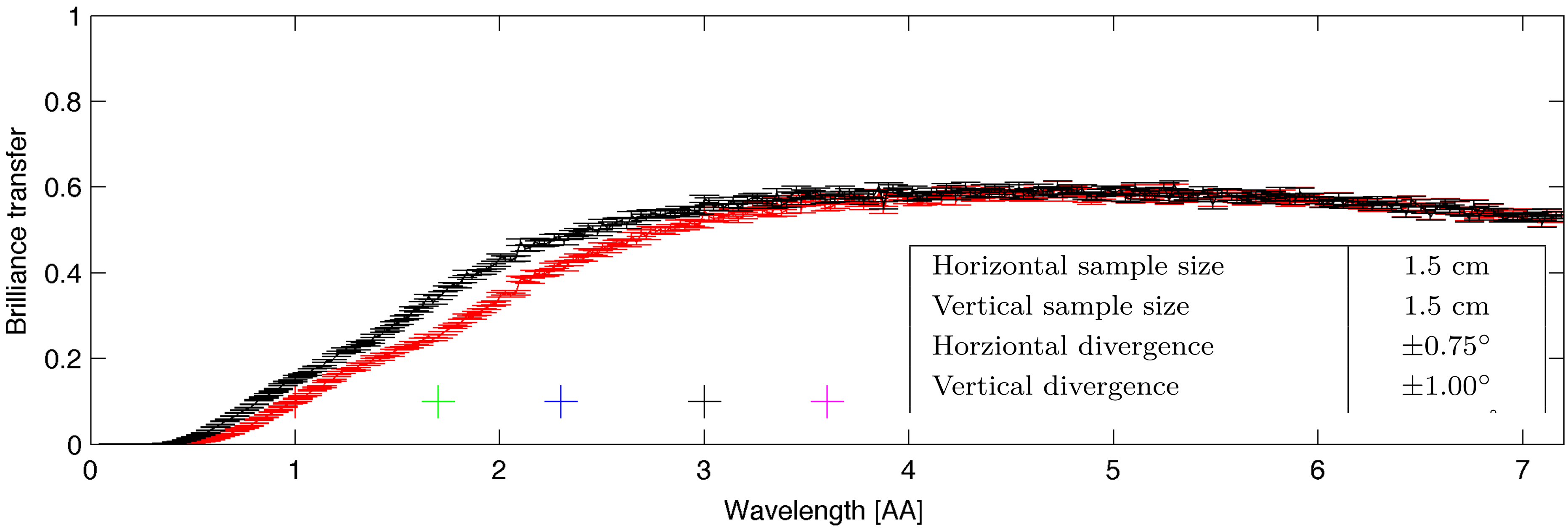
Guide Illumination



$$BT = \frac{\int_{source} B\, dA\, d\Omega\, d\lambda}{\int_{sample} B\, dA\, d\Omega\, d\lambda}$$

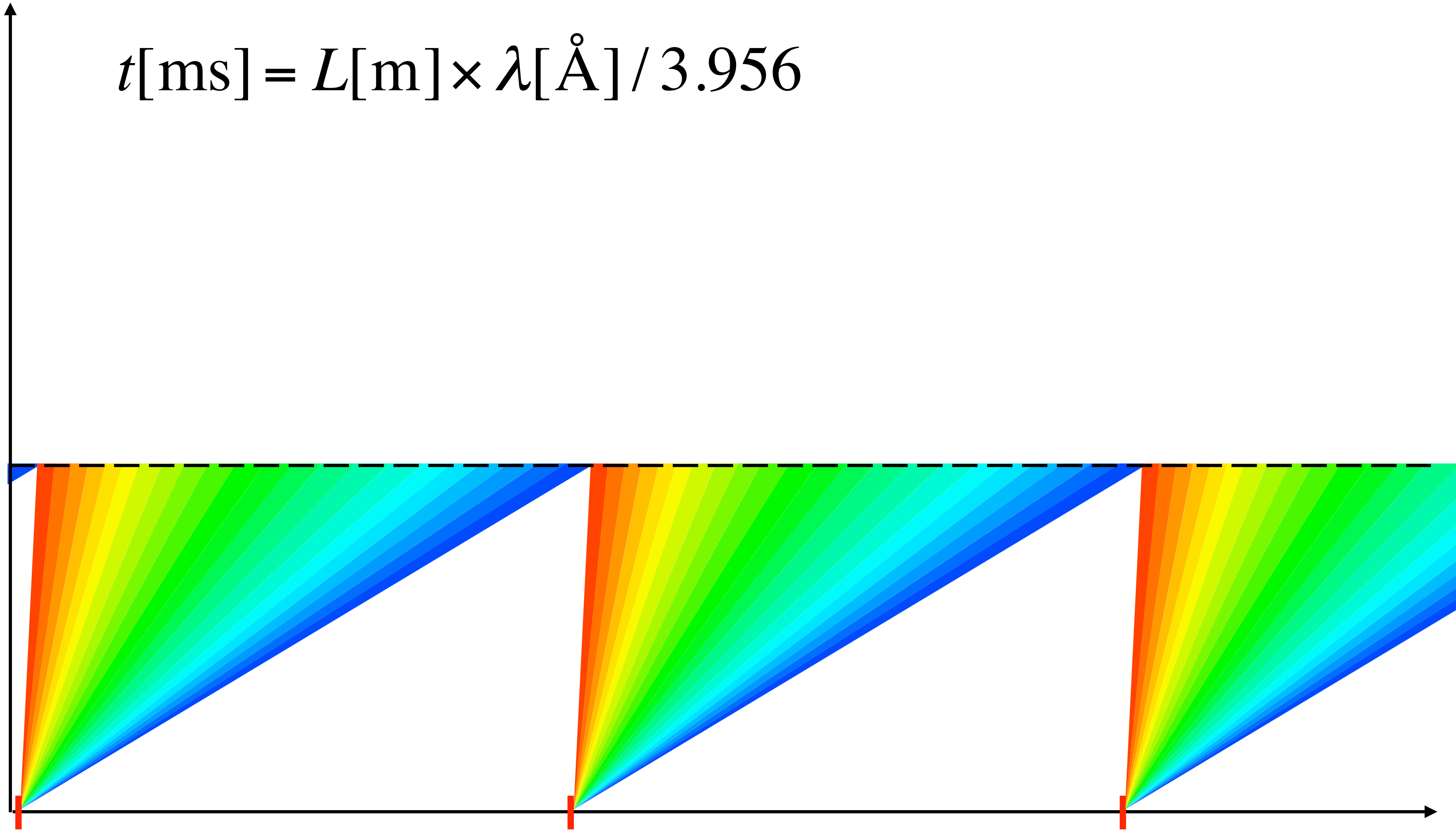
Brilliance Transfer as a Guide Design Diagnostic

McStas simulations for BIFROST spectrometer at ESS viewing 3 cm tall cold moderator



Example: ESS SANS

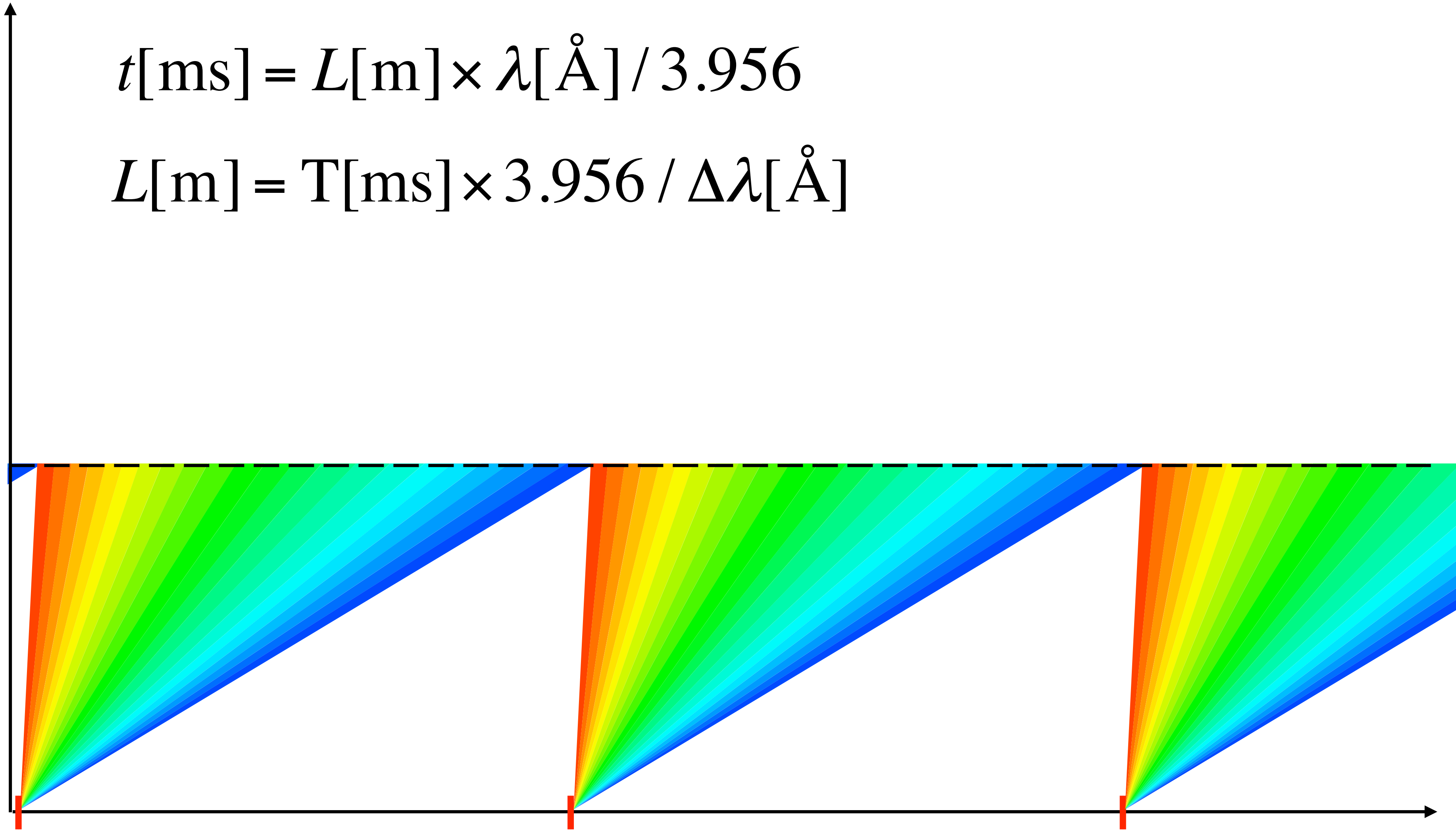
$$t[\mathrm{ms}] = L[\mathrm{m}] \times \lambda[\text{Å}] / 3.956$$



Example: ESS SANS

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

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



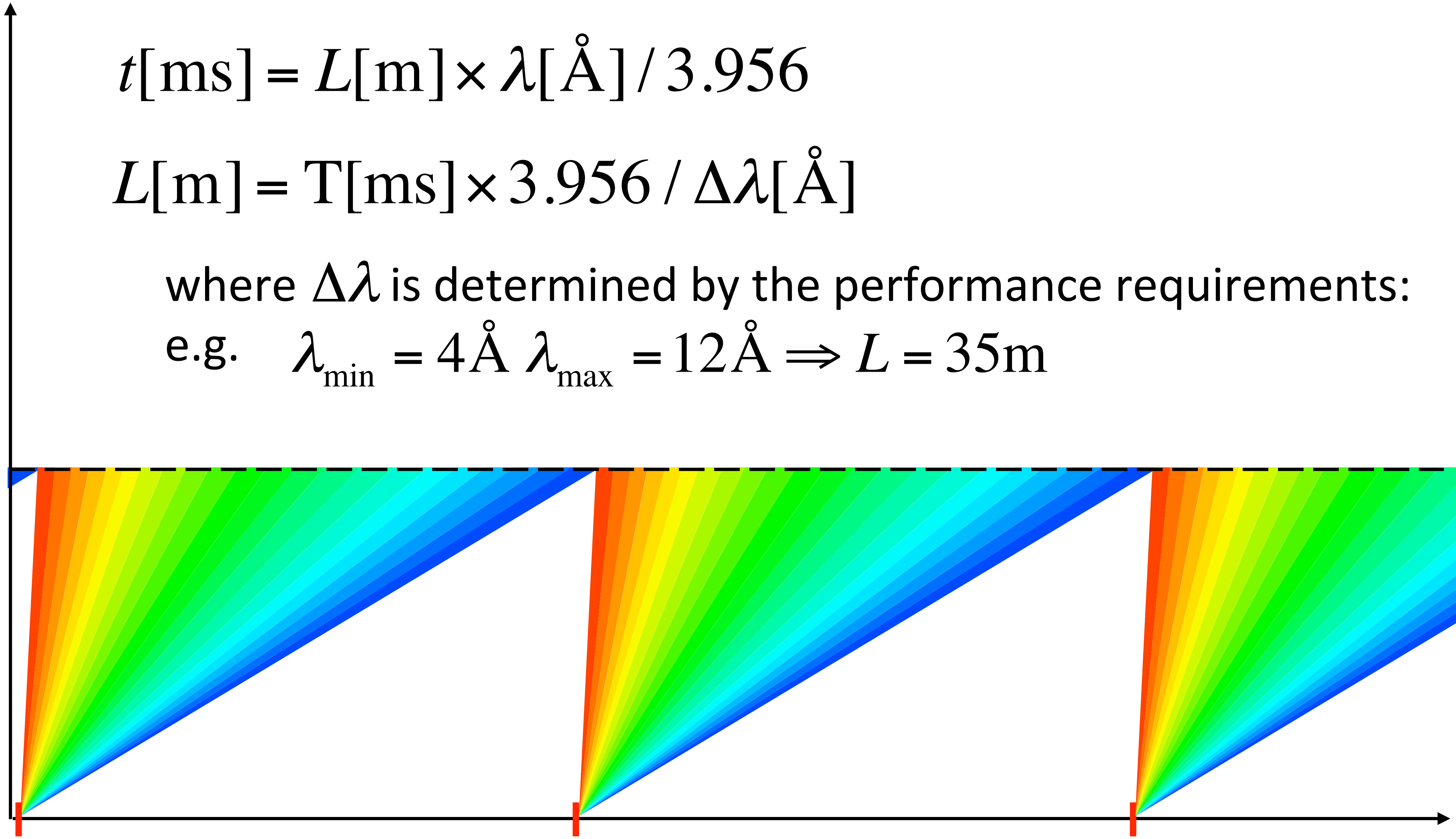
Example: ESS SANS

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

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

where $\Delta\lambda$ is determined by the performance requirements:

e.g. $\lambda_{\text{min}} = 4\text{Å}$ $\lambda_{\text{max}} = 12\text{Å} \Rightarrow L = 35\text{m}$



Example: ESS SANS

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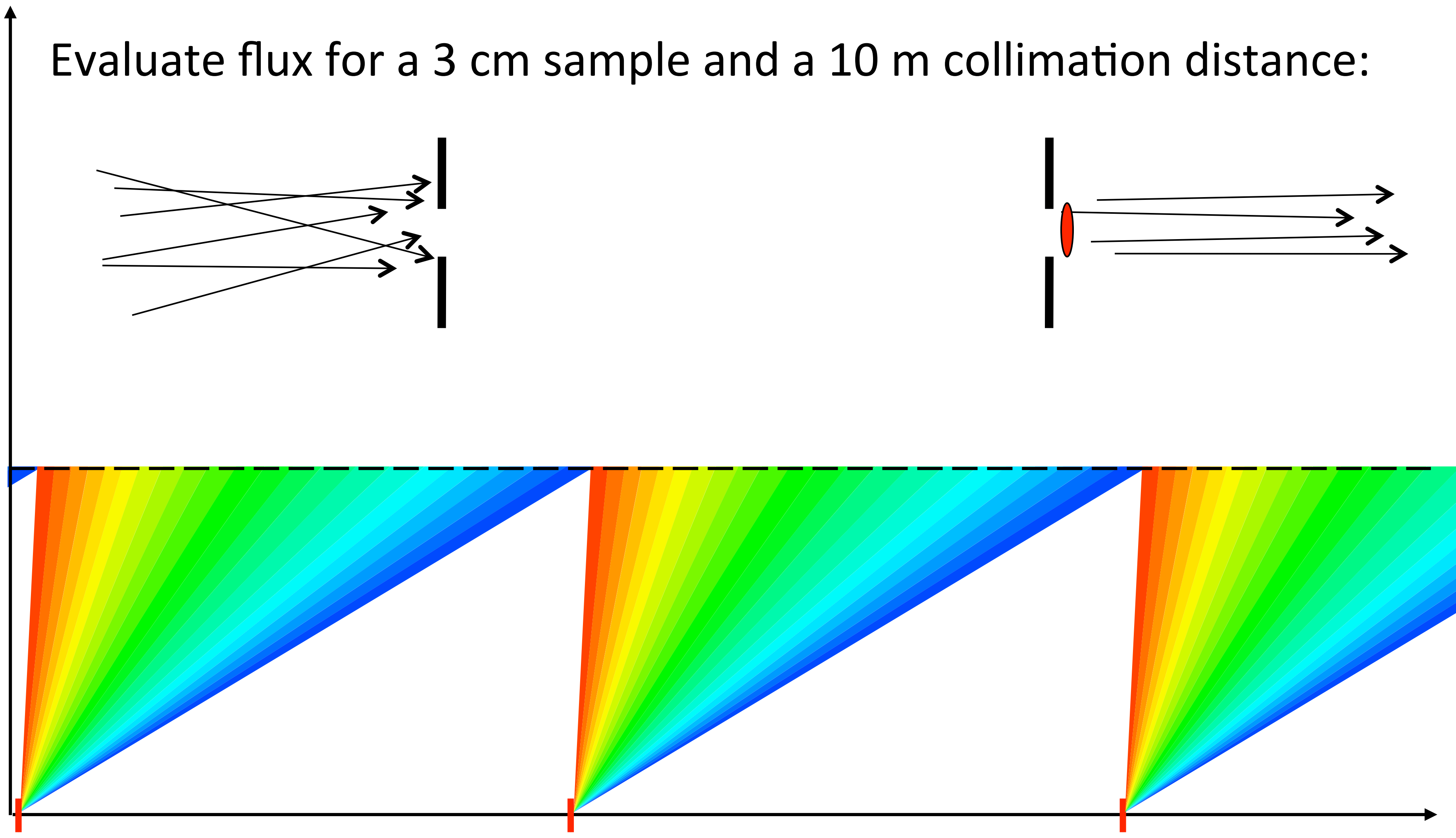
Evaluate flux for a 3 cm sample and a 10 m collimation distance:



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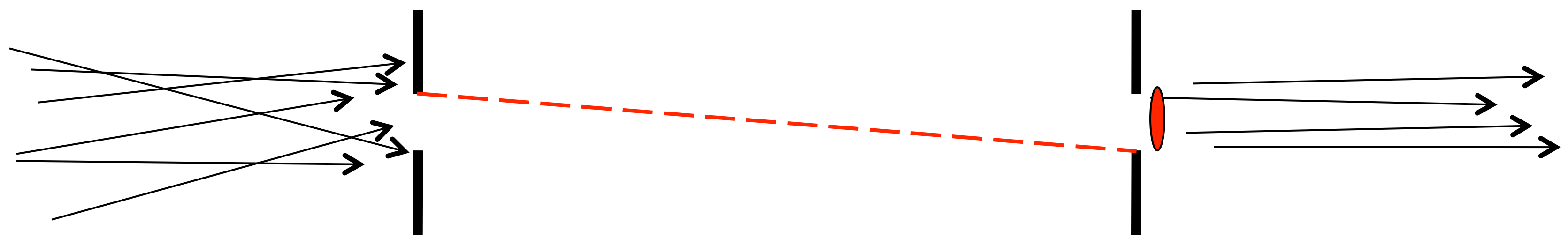

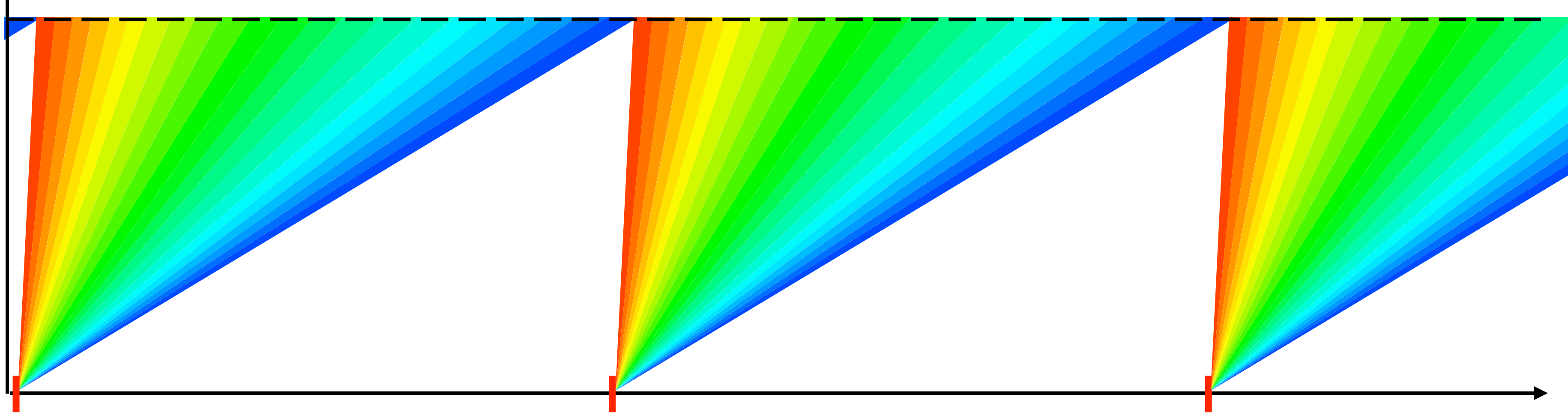

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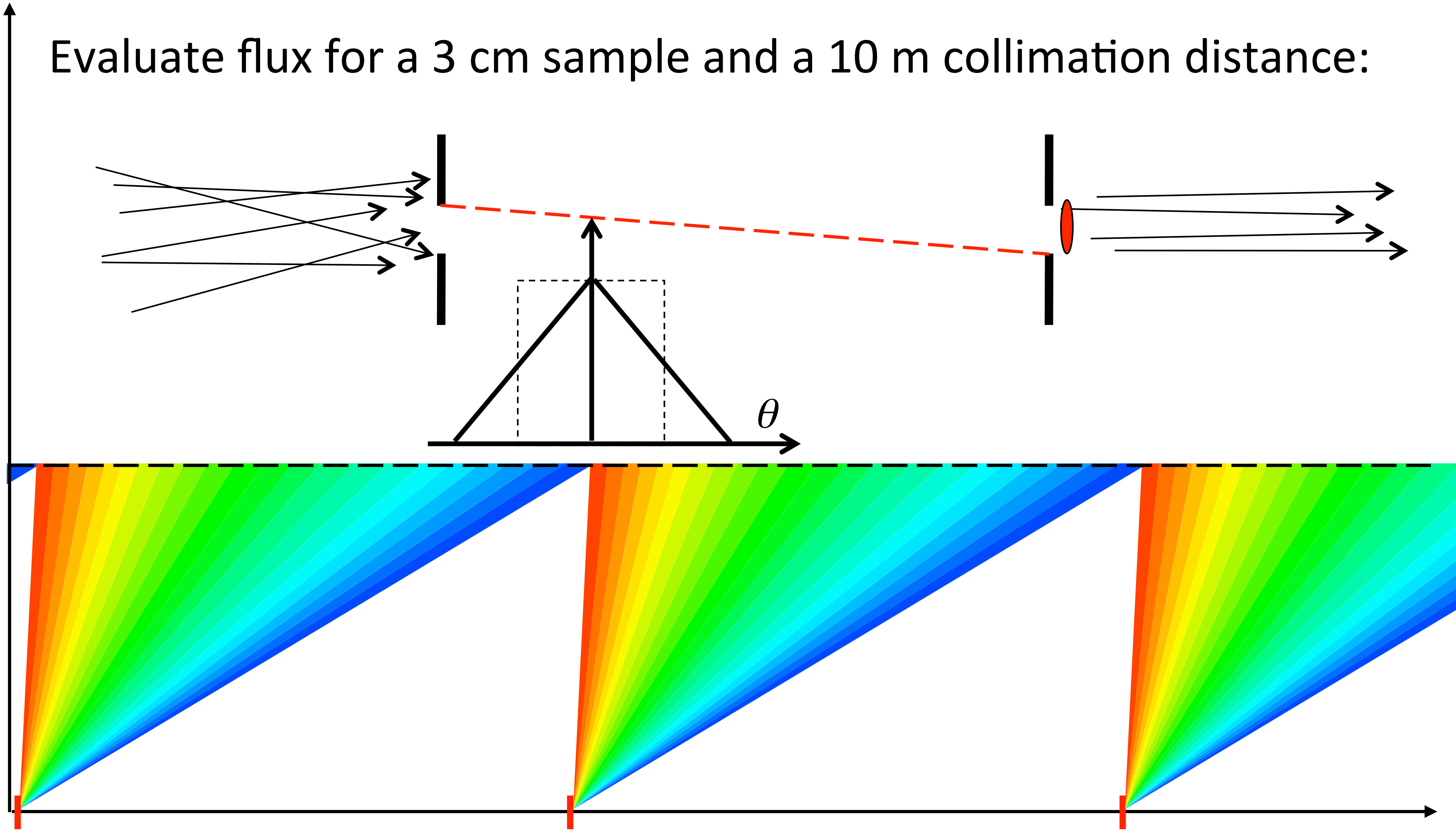

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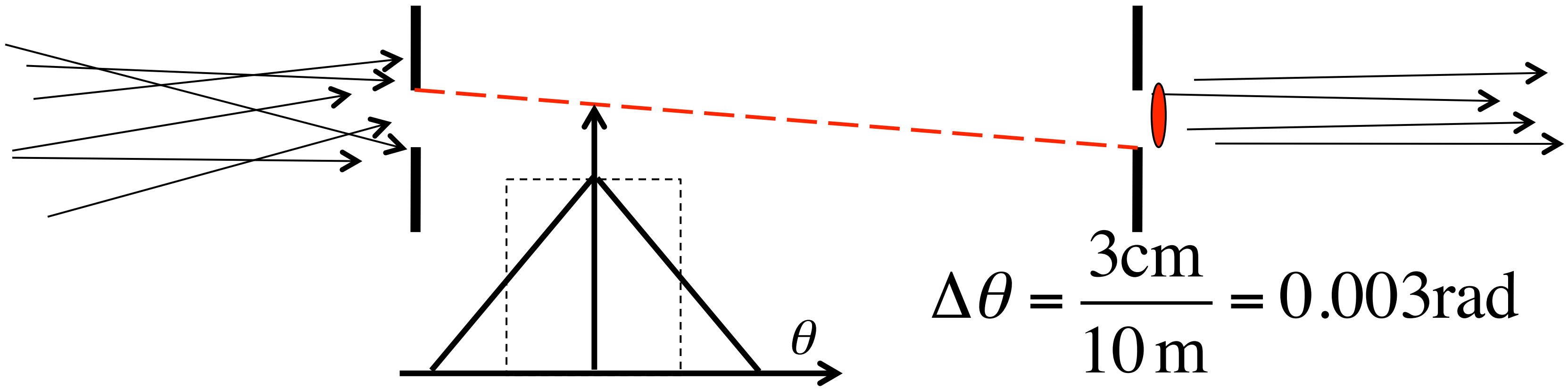
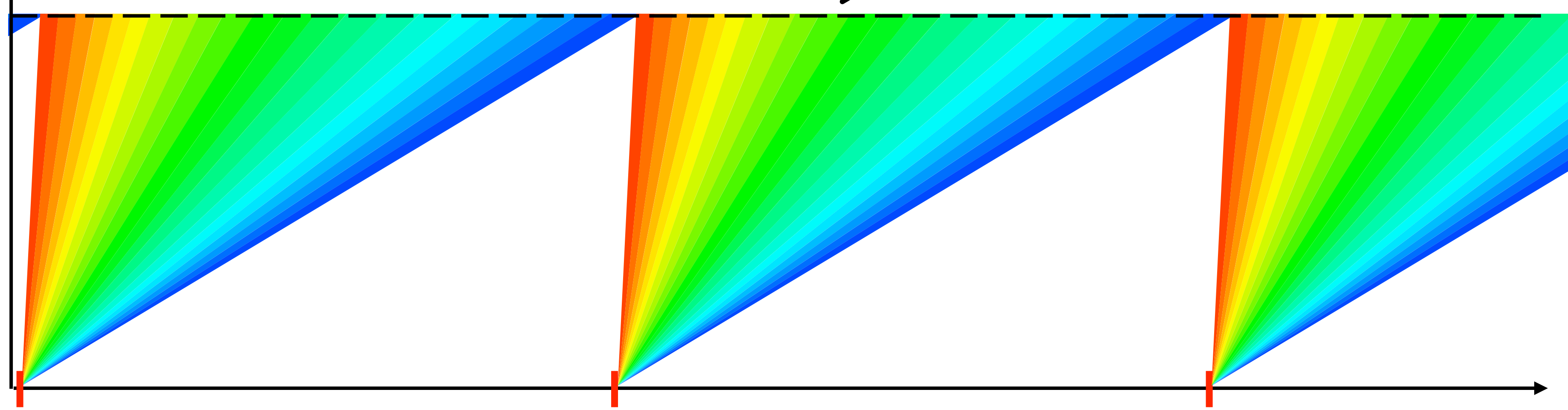


$$\Delta\theta = \frac{3\,\text{cm}}{10\,\text{m}} = 0.003\,\text{rad}$$



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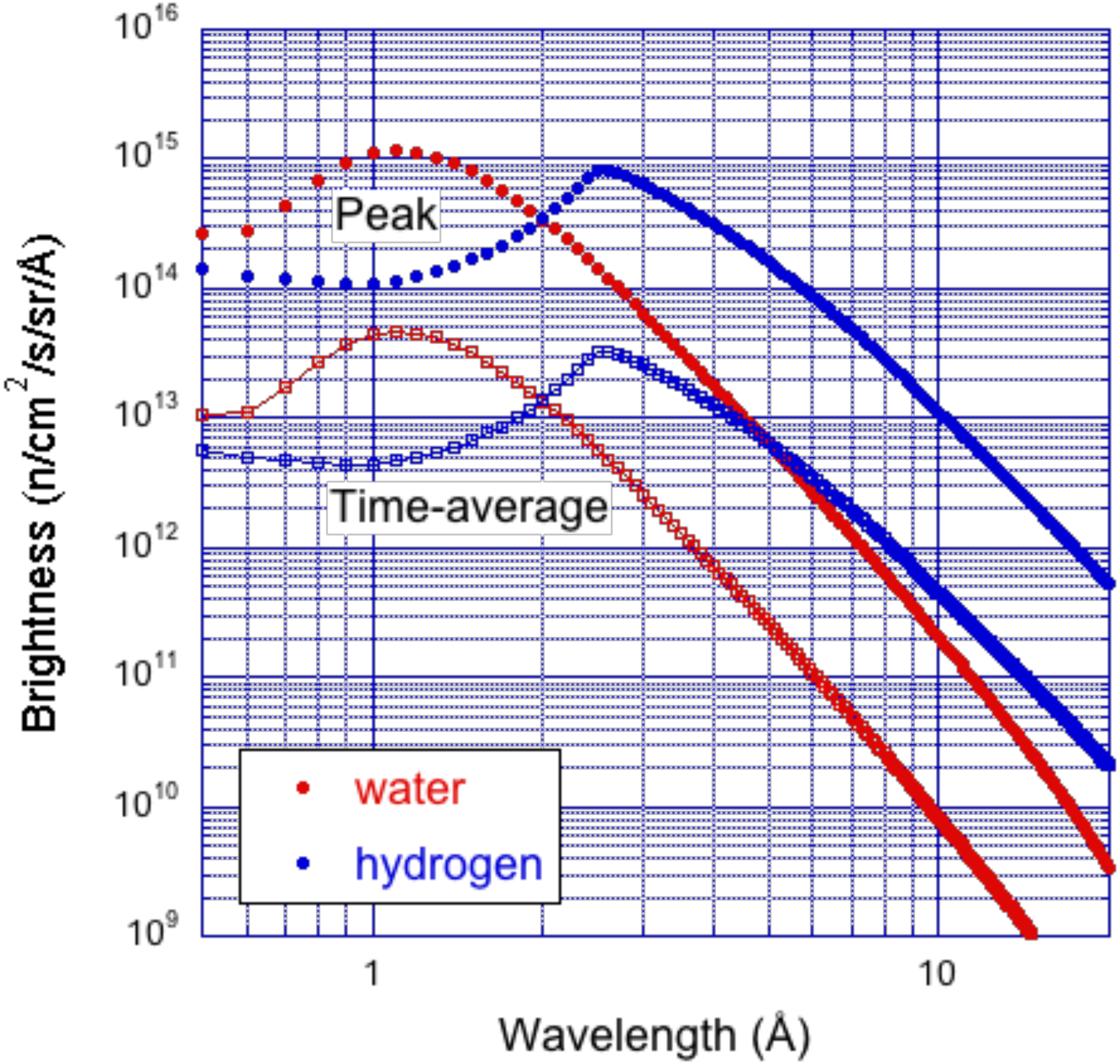
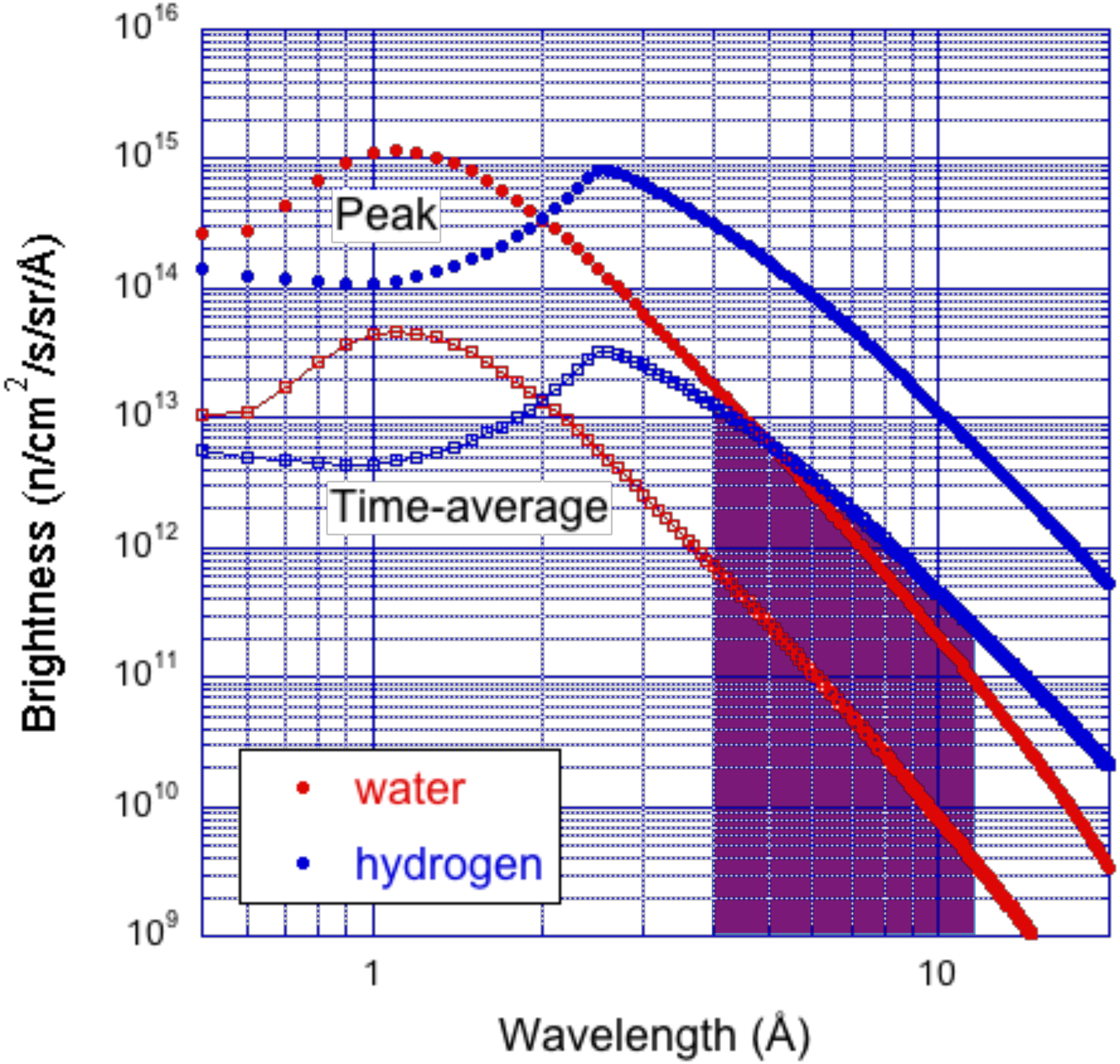


$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\, \mathrm{d}\lambda \times \Delta\Omega$$

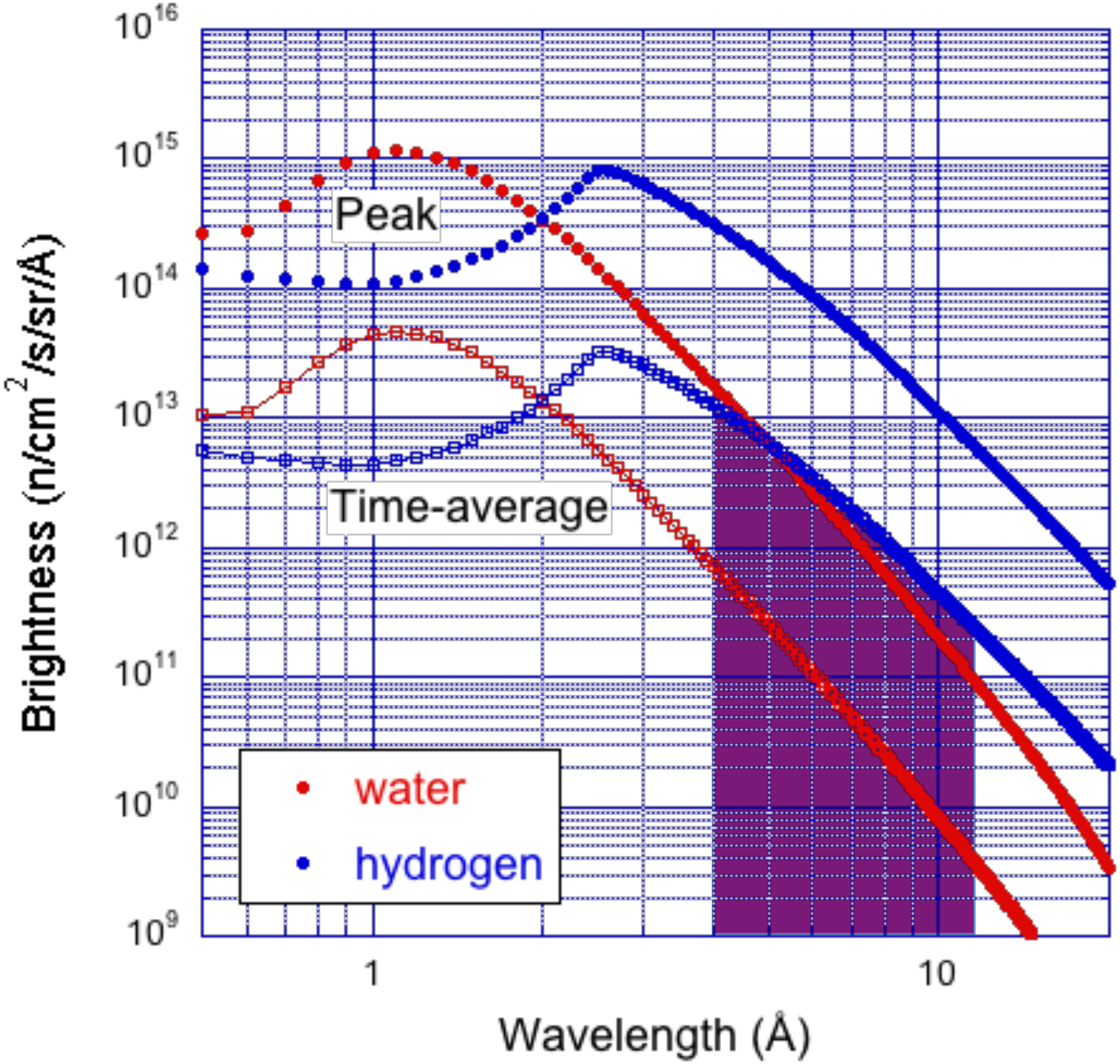
Example: ESS SANS



$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\, d\lambda \times \Delta\Omega$$

$$4\text{Å} < \lambda < 12\text{Å}$$

Example: ESS SANS



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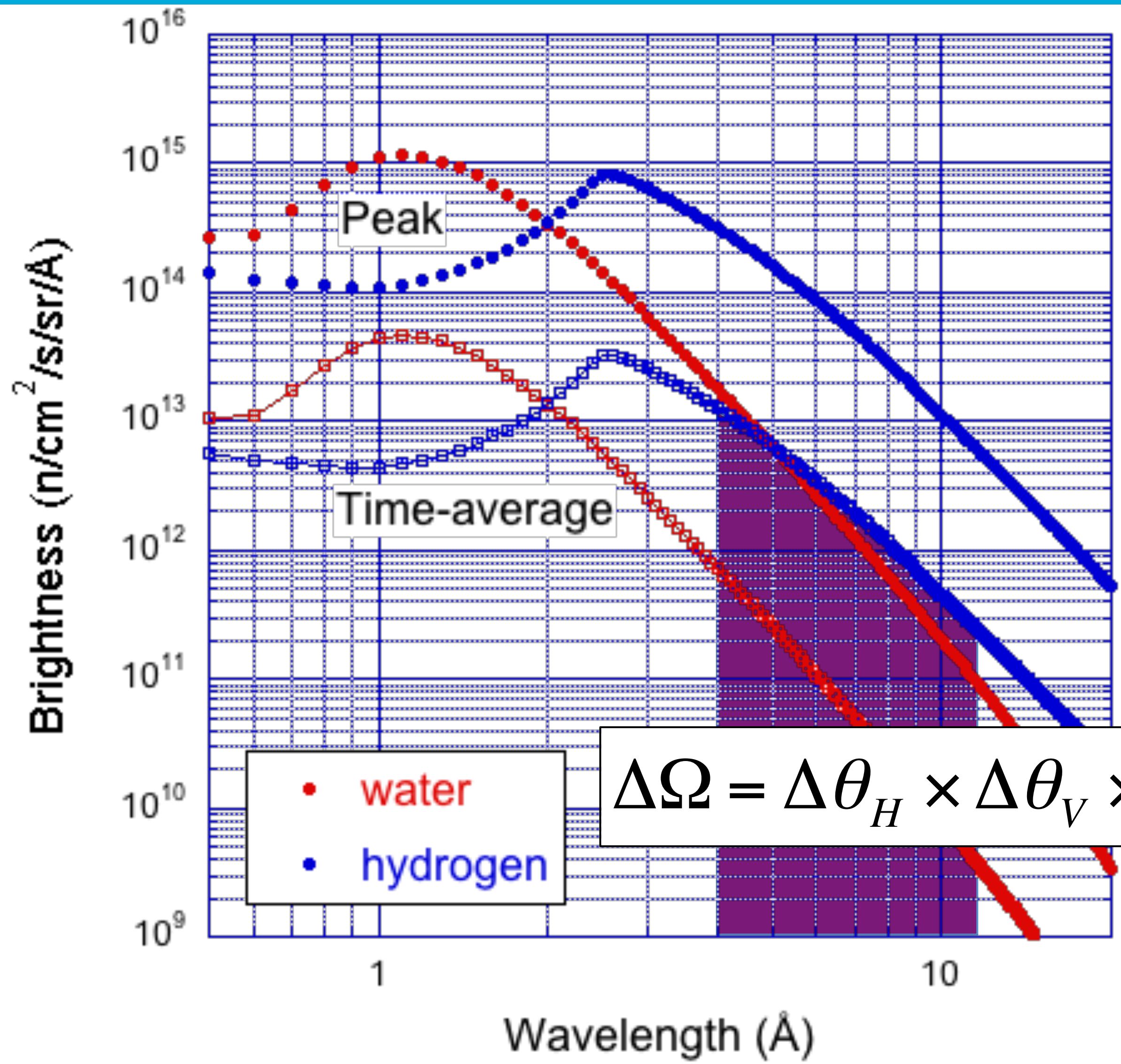
$$4\text{Å} < \lambda < 12\text{Å}$$

$$\int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\, d\lambda$$

$$\approx 2\text{E}13 \text{ n/cm}^2\text{/s/sr}$$

Example: ESS SANS



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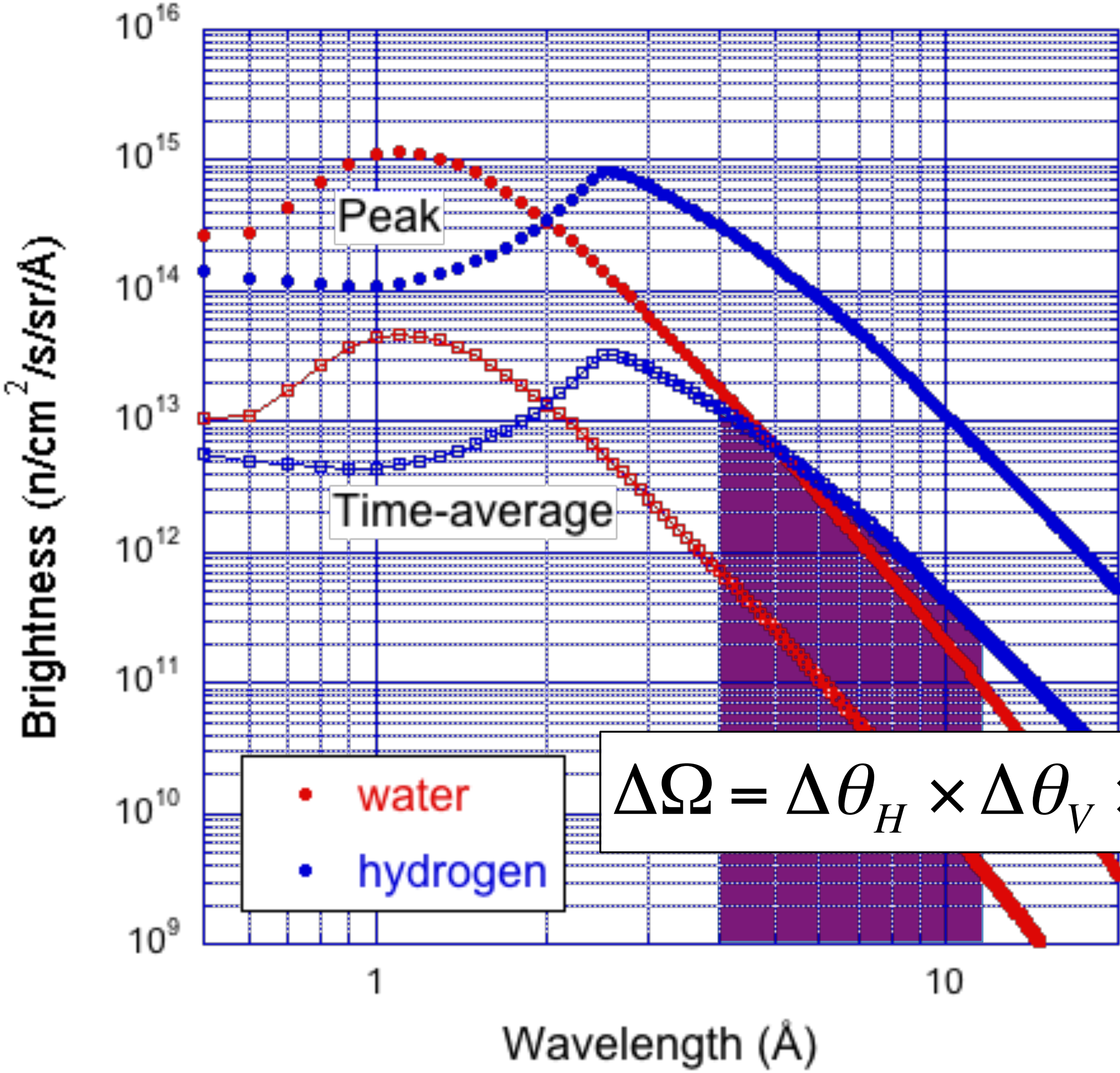
$$4\text{Å} < \lambda < 12\text{Å}$$

$$\int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, \mathrm{d}\lambda \approx 2\text{E13 n/cm}^2\text{/s/sr}$$

$$\Delta\Omega = \Delta\theta_H \times \Delta\theta_V \times \mathrm{BT} = 0.003^2\,\mathrm{sr} \times 0.5$$

Example: ESS SANS



$$\Phi = \int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, d\lambda \times \Delta\Omega$$

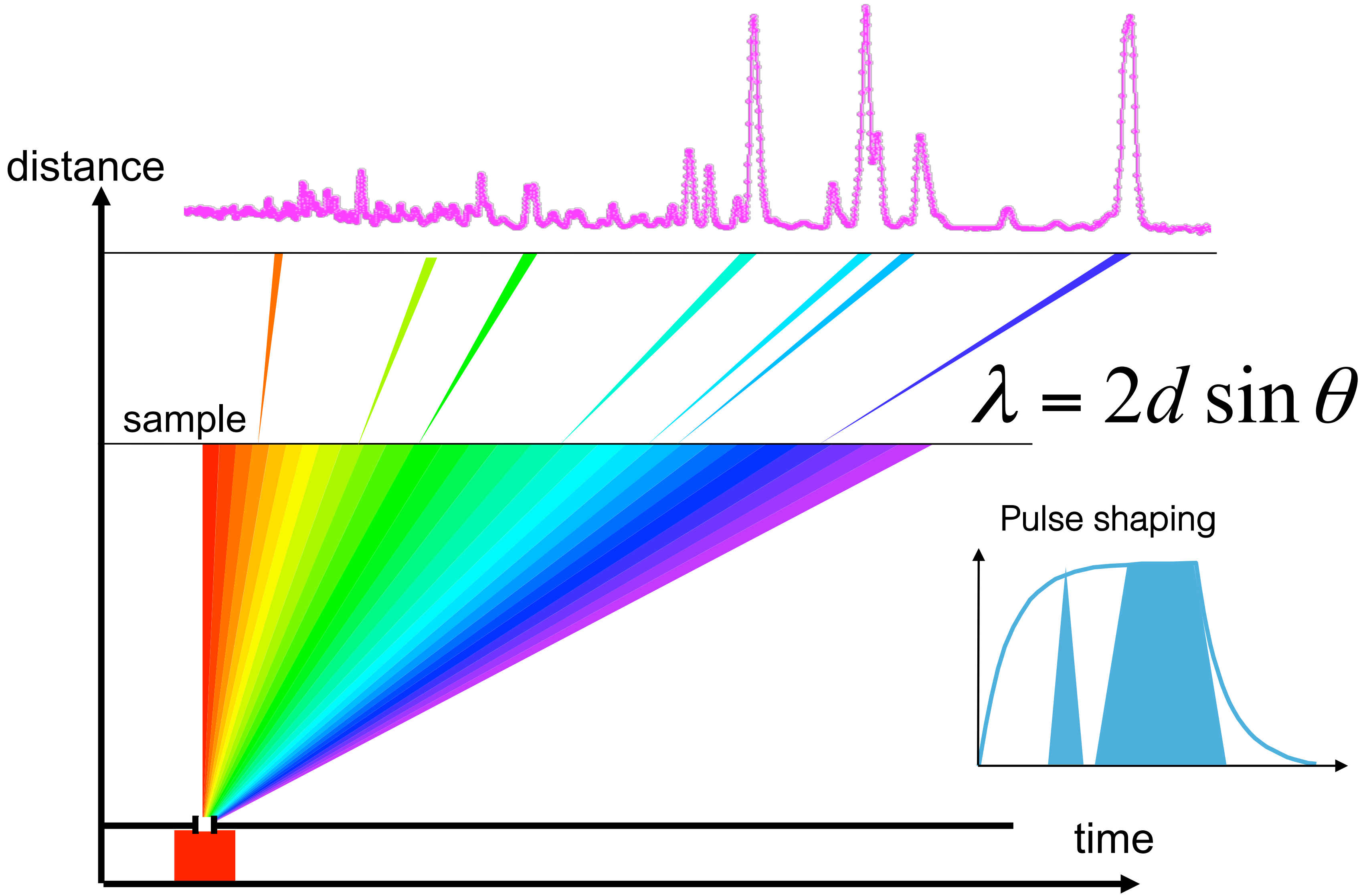
$$4Å < \lambda < 12Å$$

$$\int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, d\lambda \approx 2E13 \text{ n/cm}^2\text{/s/sr}$$

$$\Delta\Omega = \Delta\theta_H \times \Delta\theta_V \times BT = 0.003^2 \text{sr} \times 0.5$$

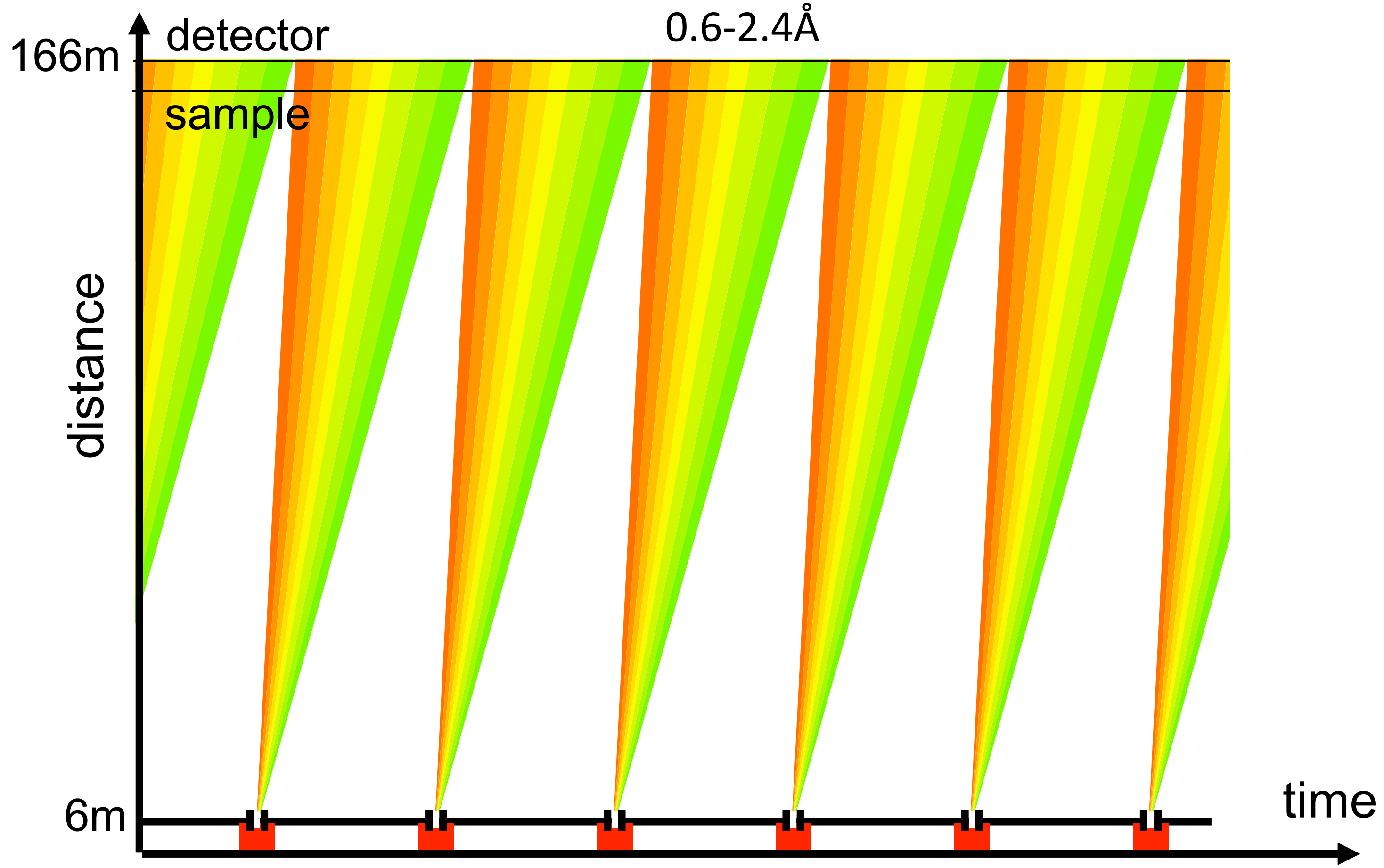
$$\Phi \approx 9E7 \text{ n/cm}^2\text{/s}$$

Example: ESS Powder Diffractometer



$$\lambda = 2d\sin\theta$$

Example: ESS Powder Diffractometer



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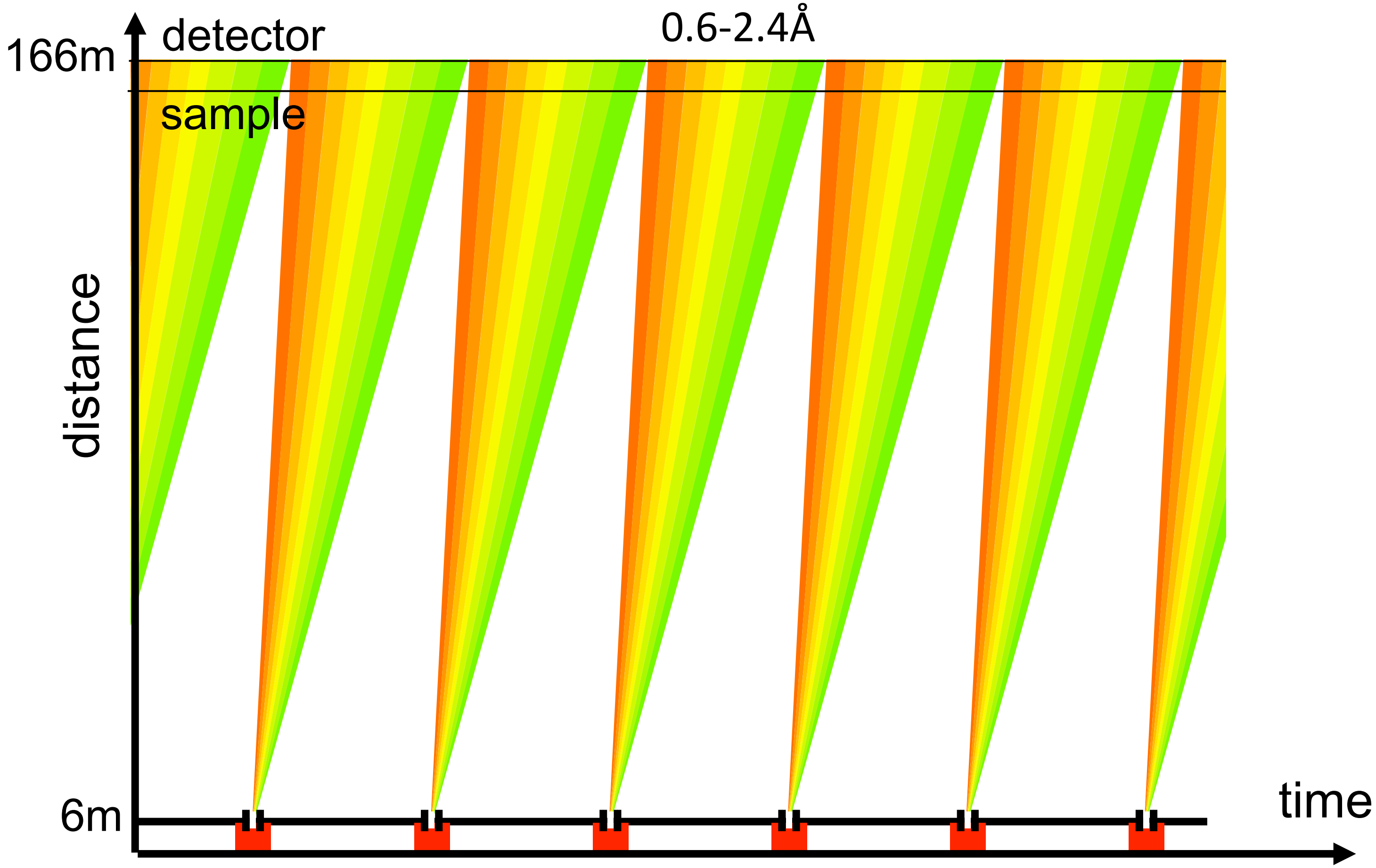
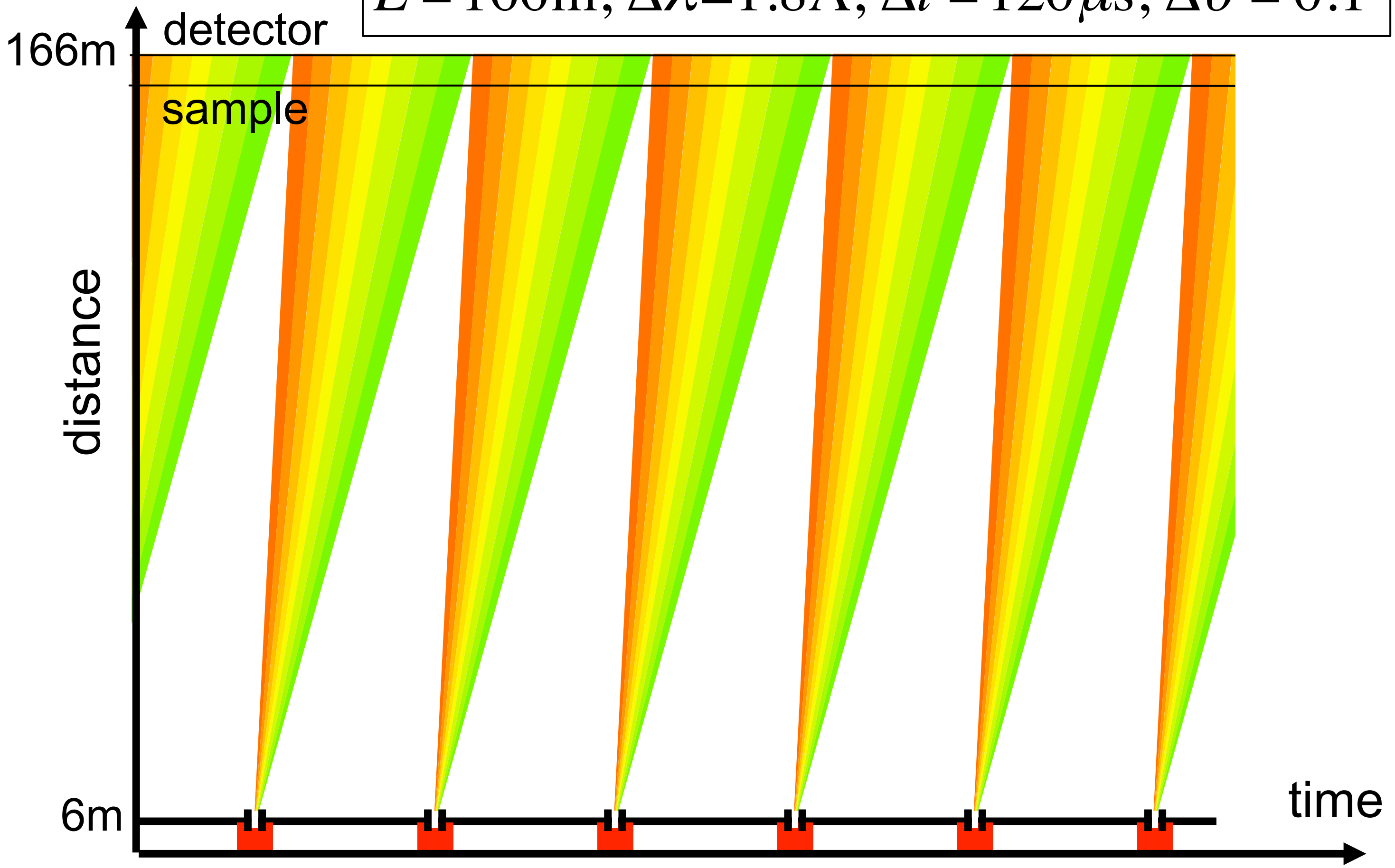
$$t[\text{ms}] = L[\text{m}] \times \lambda[\text{Å}] / 3.956$$



Example: ESS Powder Diffractometer

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

$$L = 166\mathrm{m},\ \Delta\lambda = 1.8\text{Å},\ \Delta t = 120\mu\mathrm{s},\ \Delta\theta = 0.1^{\circ}$$



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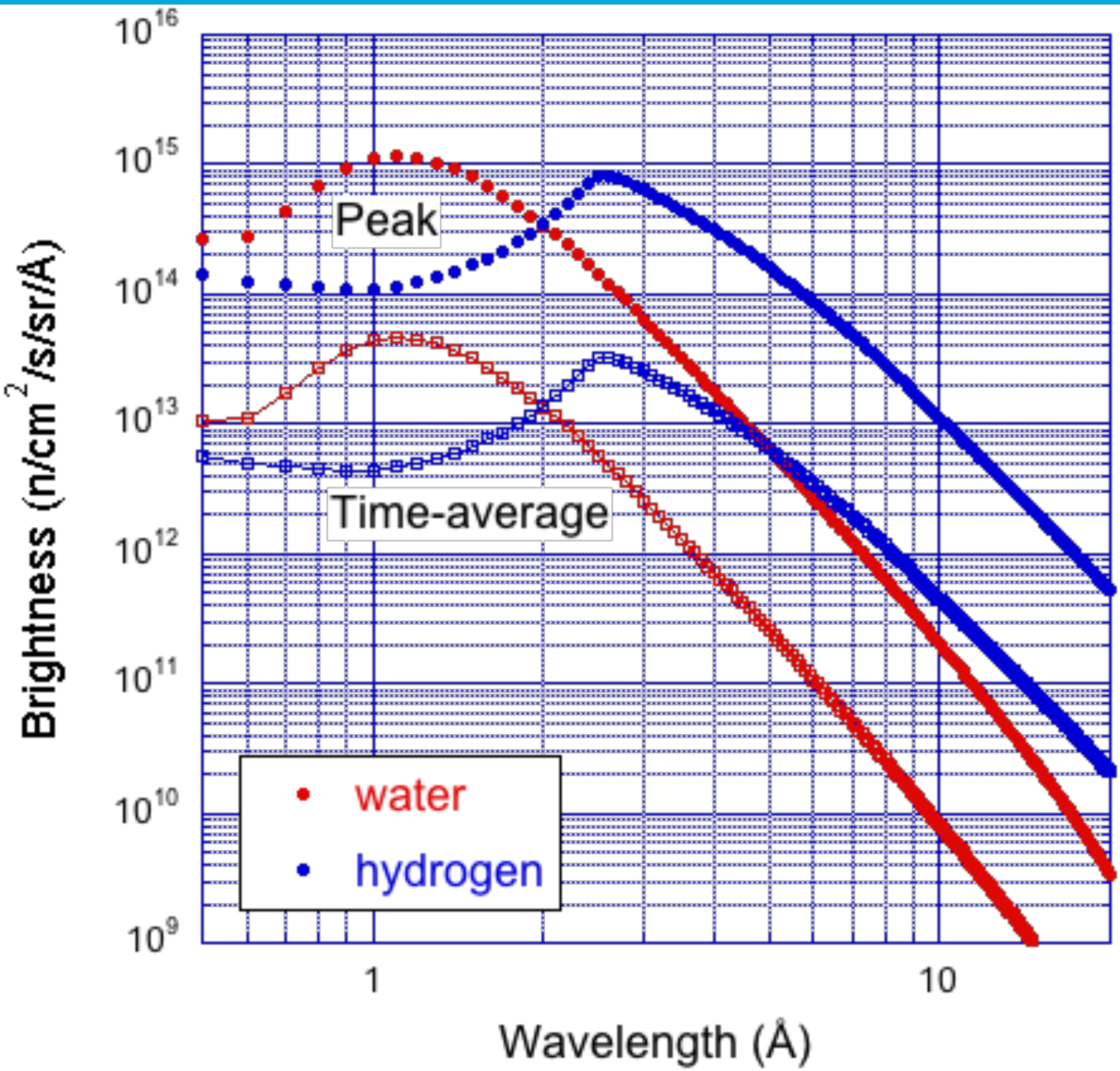

$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\,\mathrm{d}\lambda \times \Delta\Omega$$

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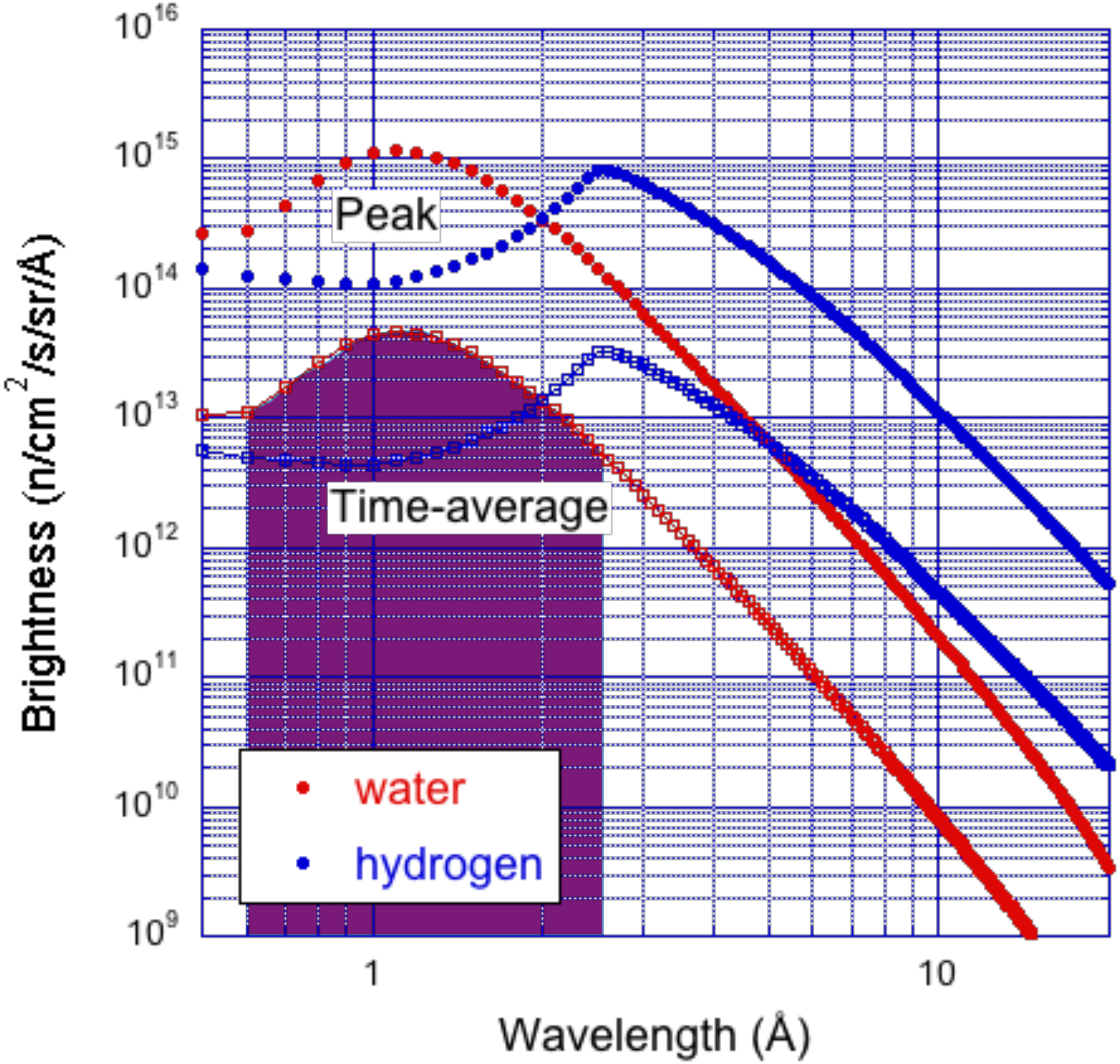
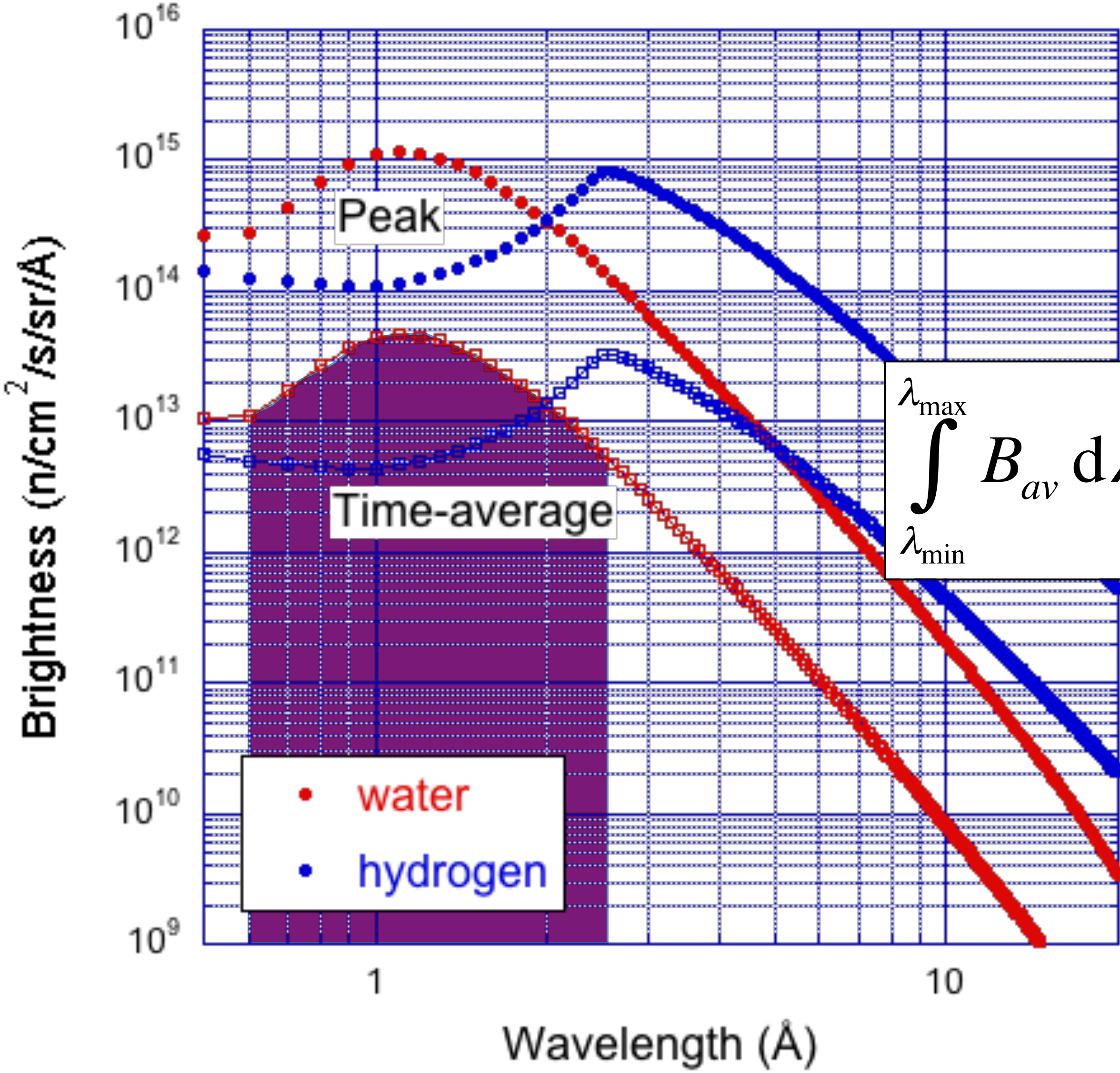


$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\, \mathrm{d}\lambda \times \Delta\Omega$$

$$0.6\text{Å} < \lambda < 2.4\text{Å}$$

Example: ESS Powder Diffractometer



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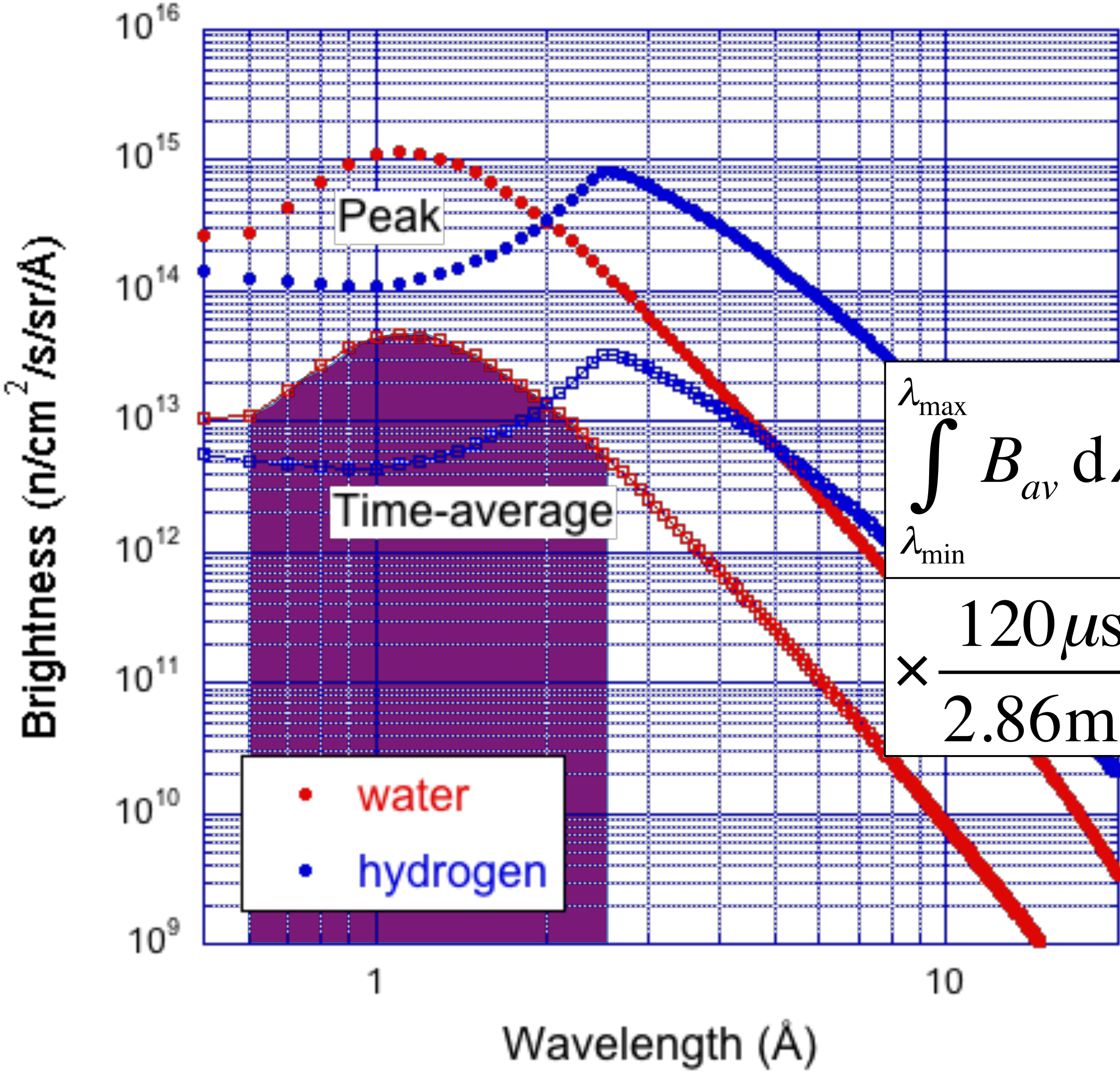
$$0.6Å < \lambda < 2.4Å$$

$$\int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, d\lambda = 4.7\times 10^{13}\ \text{n/cm}^2\text{/s/sr}$$

Example: ESS Powder Diffractometer



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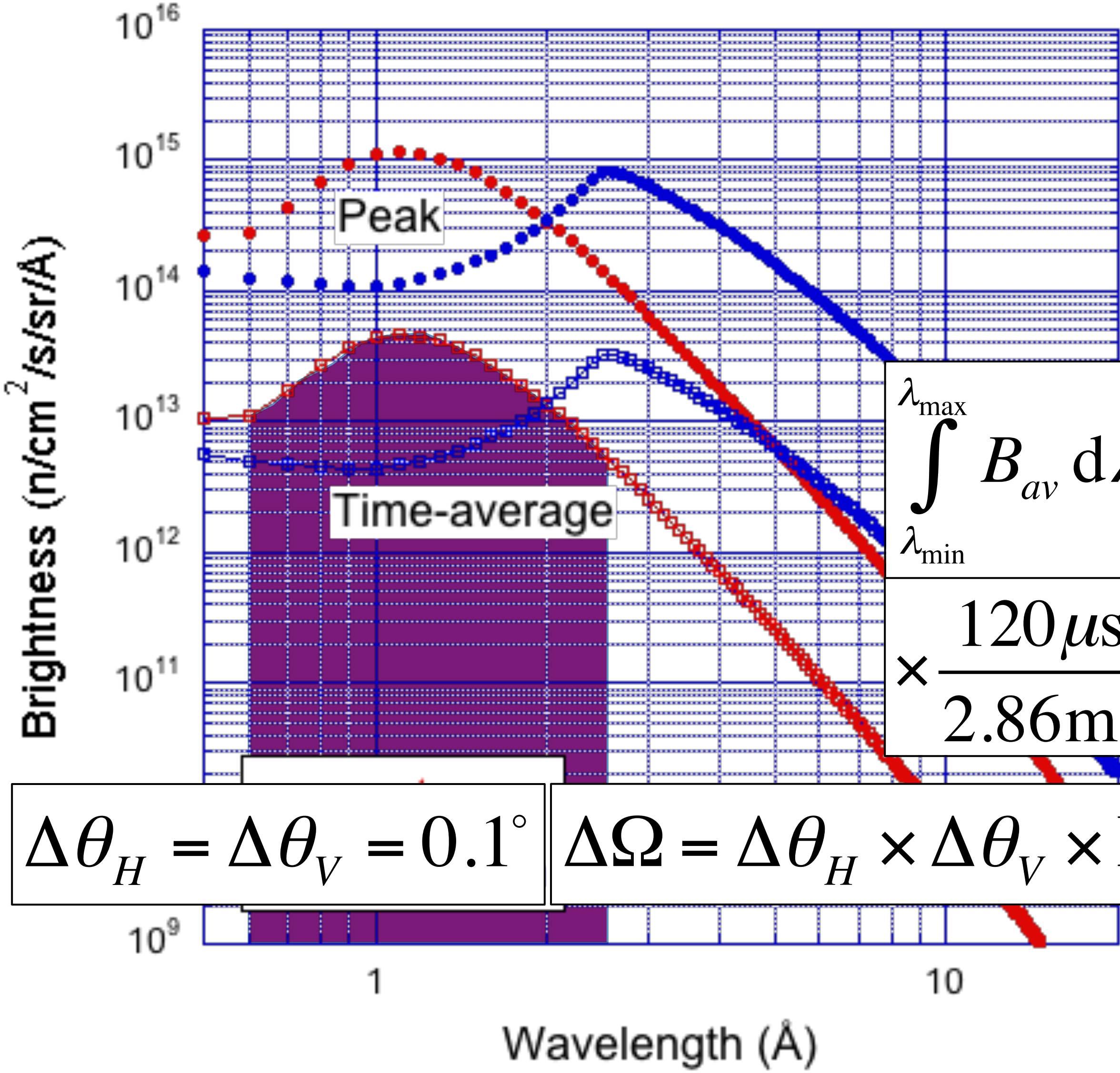
$$\times \frac{120\mu s}{2.86\text{ms}} = 2.0 \times 10^{12}\ \text{n/cm}^2\text{/s/sr}$$

Example: ESS Powder Diffractometer



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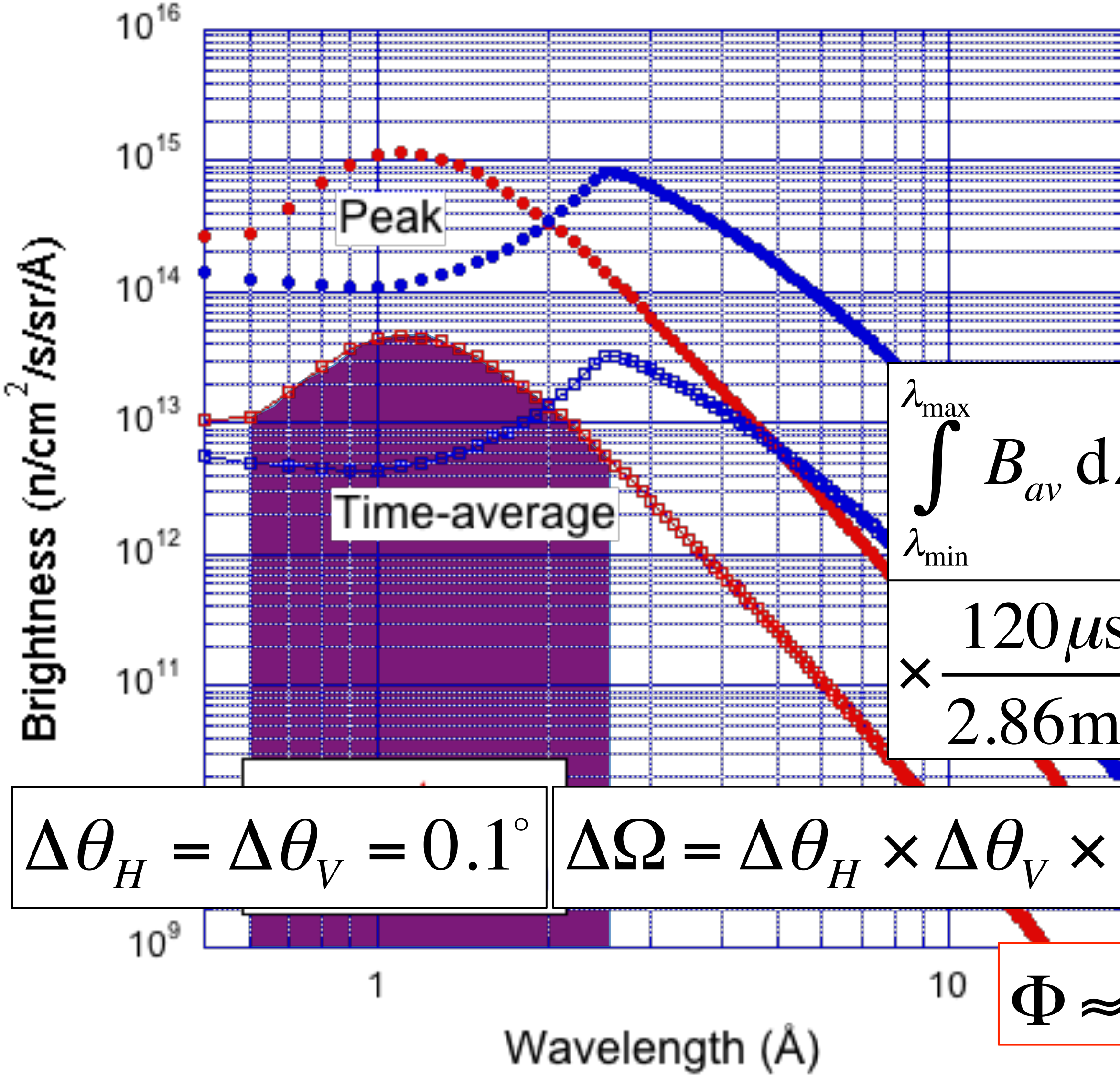
$$\Delta\theta_H = \Delta\theta_V = 0.1^\circ$$

$$\Delta\Omega = \Delta\theta_H \times \Delta\theta_V \times \text{BT} = 0.00175^2\,\text{sr} \times 0.5$$

Example: ESS Powder Diffractometer



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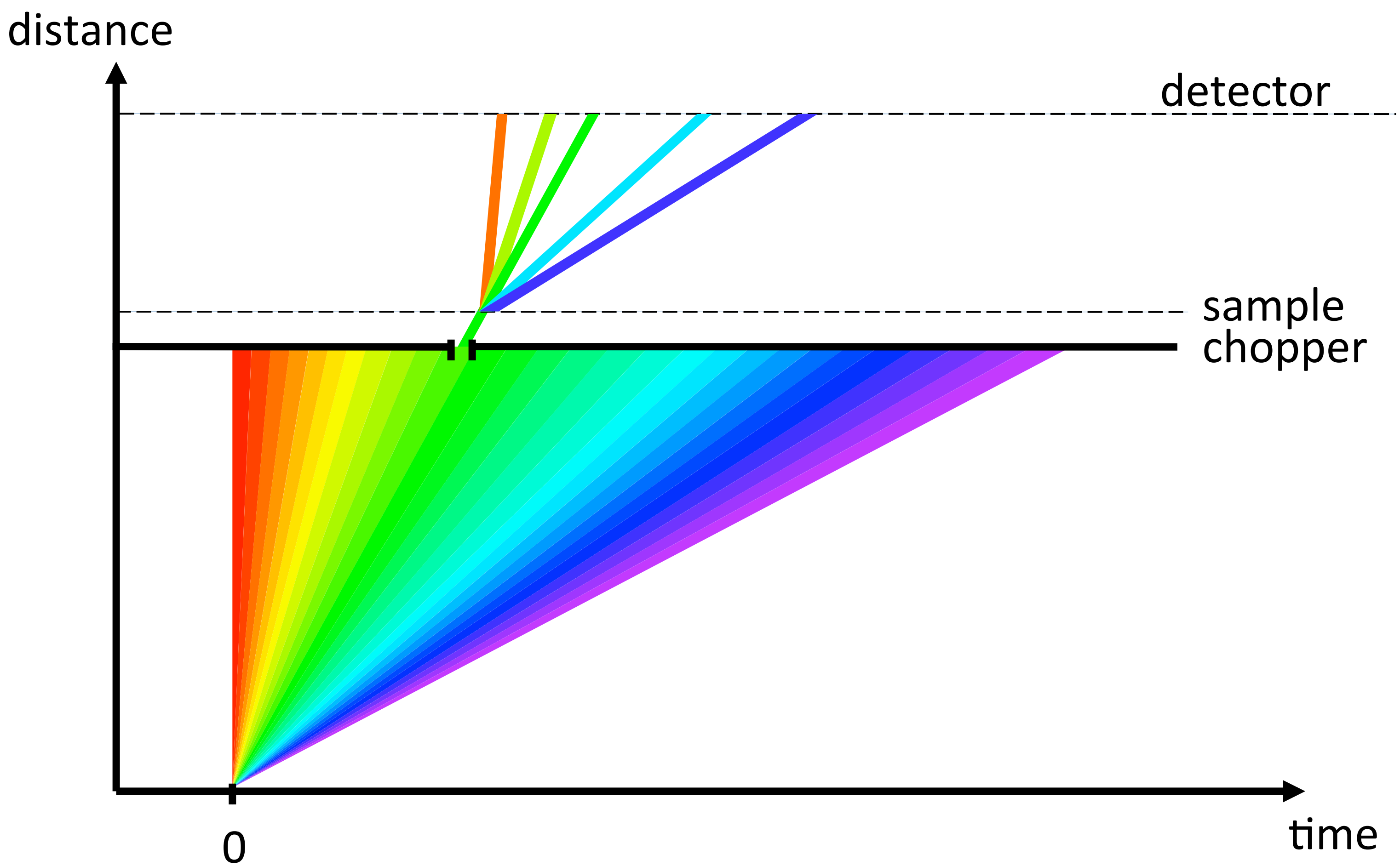
$$\Delta\Omega = \Delta\theta_H \times \Delta\theta_V \times \text{BT} = 0.00175^2\,\text{sr} \times 0.5$$

$$\Phi \approx 3\times 10^{6}\ \text{n/cm}^2\text{/s}$$

Example: SNS STS Cold Chopper Spectrometer

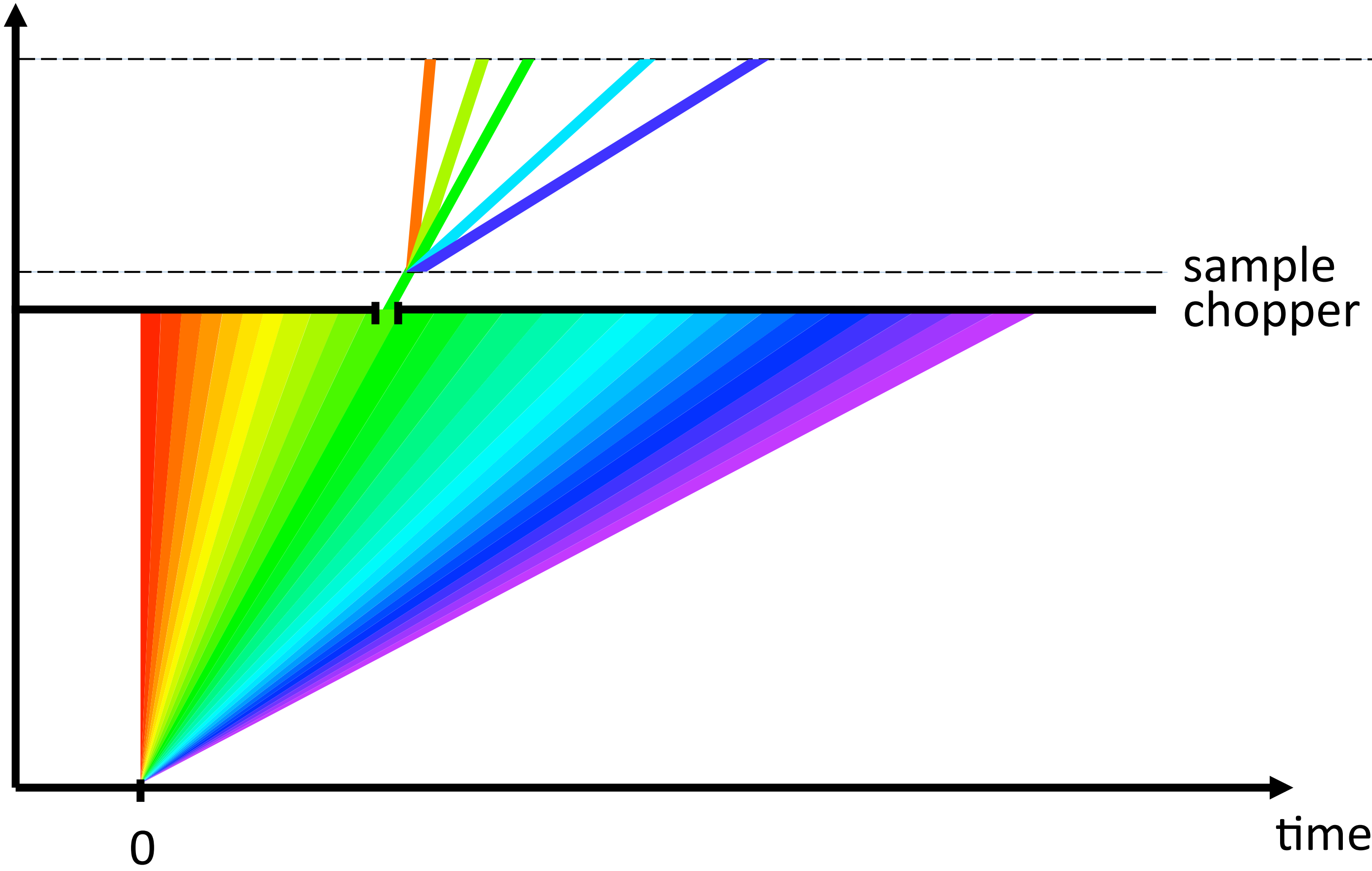
$$t[\mathrm{ms}] = L[\mathrm{m}] \times \lambda[\text{Å}] / 3.956$$



Example: SNS STS Cold Chopper Spectrometer

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

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



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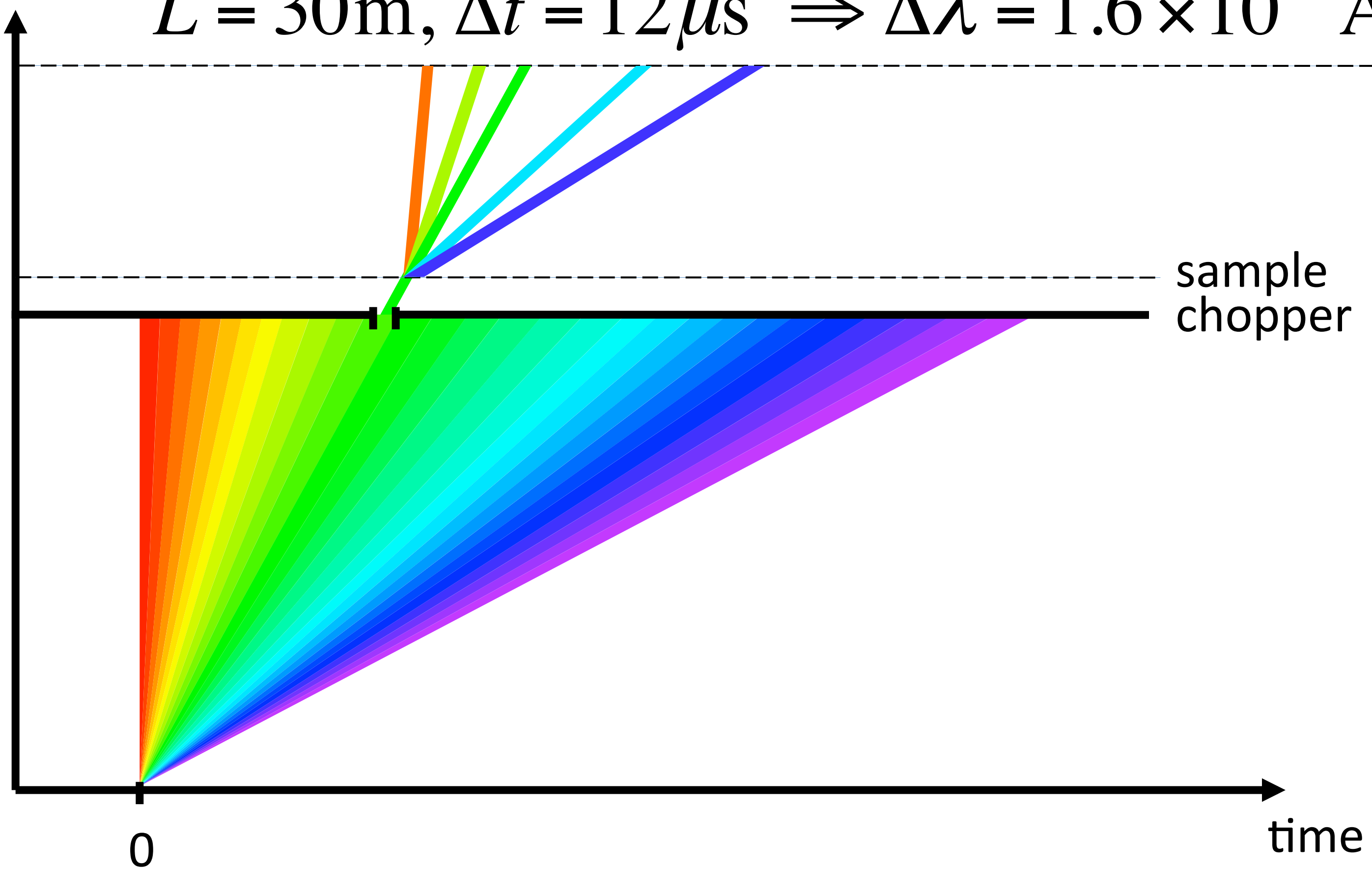
$$t[\text{ms}] = L[\text{m}] \times \lambda[\text{Å}] / 3.956$$

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

$$L = 30\text{m},\ \Delta t = 12\mu s \ \Rightarrow \Delta\lambda = 1.6 \times 10^{-3}\,\text{Å}$$



Example: SNS STS Cold Chopper Spectrometer

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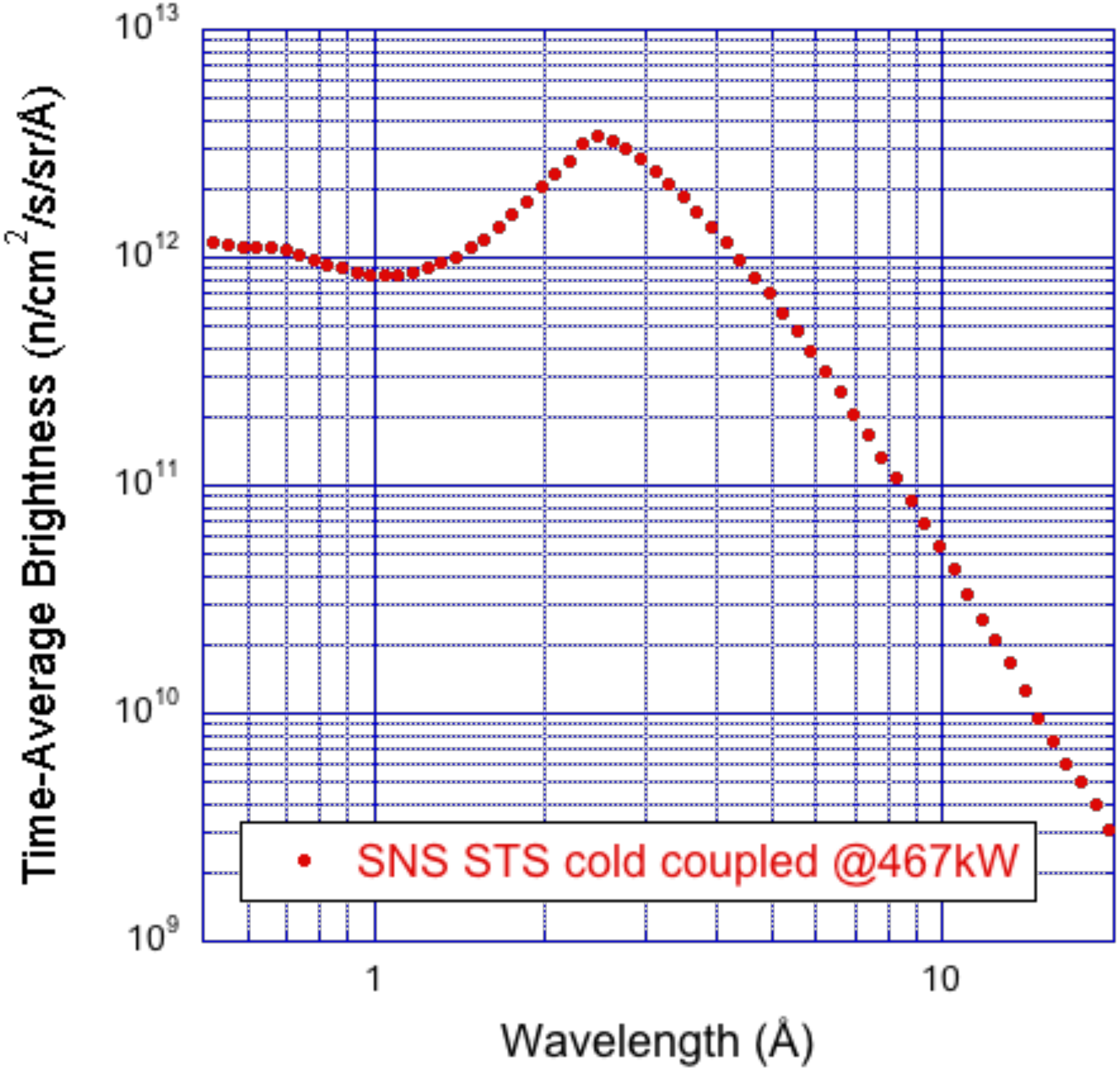

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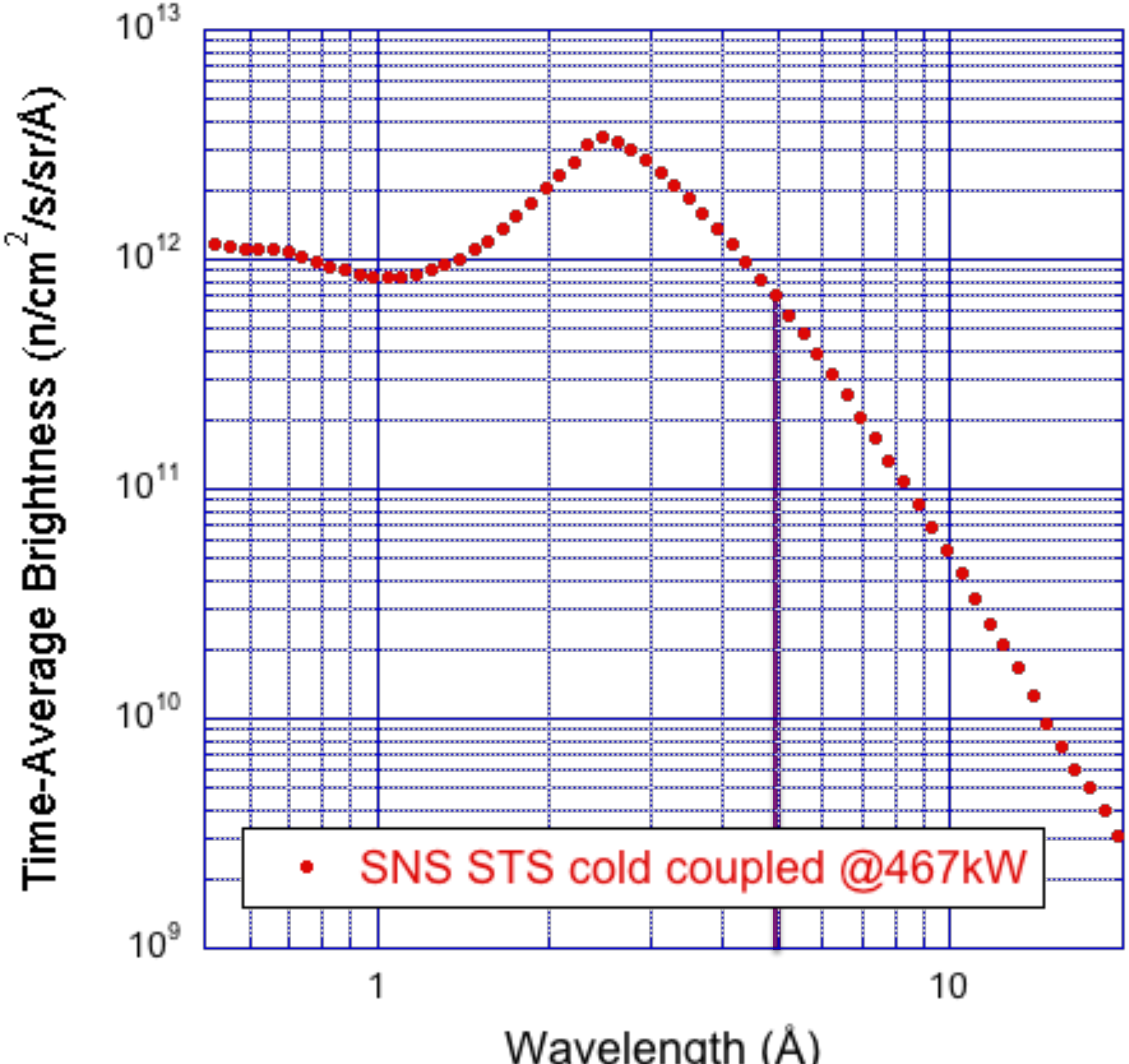

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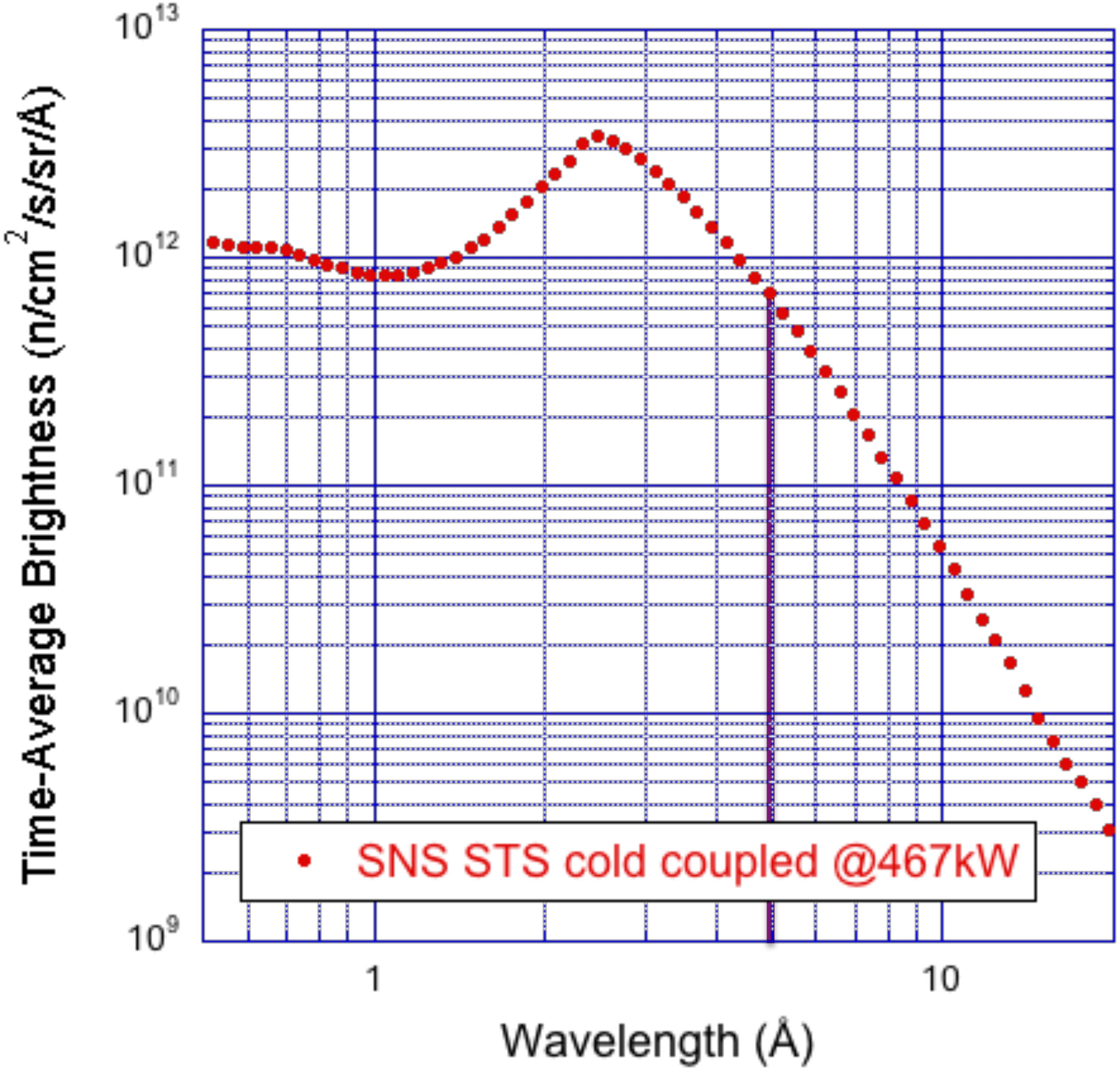

$$\Phi = \int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, \mathrm{d}\lambda \times \Delta\Omega$$

$$\Delta\lambda = 1.6\times10^{-3}\ \text{Å}$$

$$\int_{\lambda_{min}}^{\lambda_{max}} B_{av}\, \mathrm{d}\lambda \text{ at } \lambda = 5\text{Å}$$

$$\approx 1.1\times10^{9}\ \text{n/cm}^2\text{/s/sr}$$

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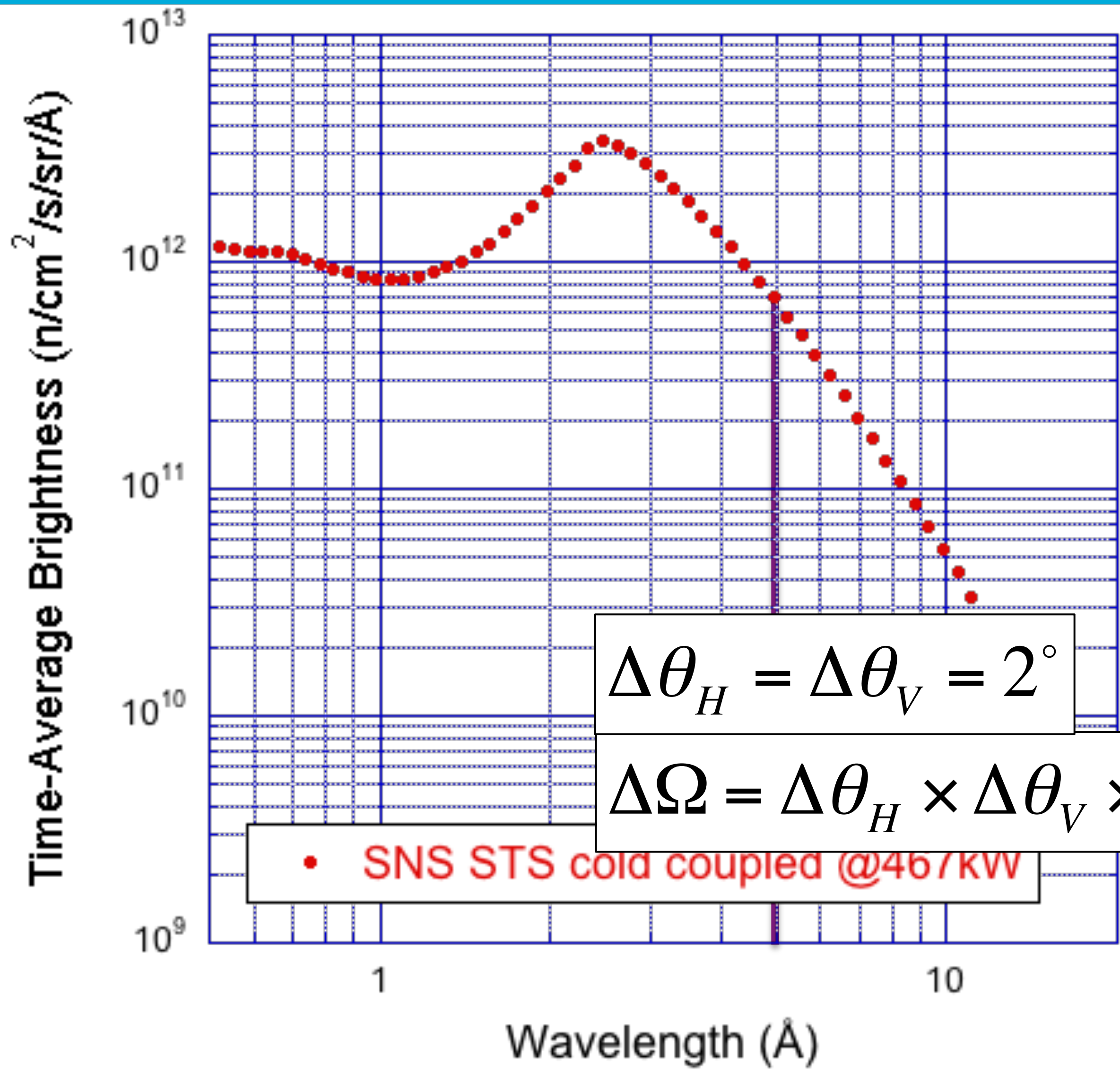

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$$\approx 1.1 \times 10^{9}\ \text{n/cm}^2\text{/s/sr}$$

$$\Delta\theta_H = \Delta\theta_V = 2^{\circ}$$

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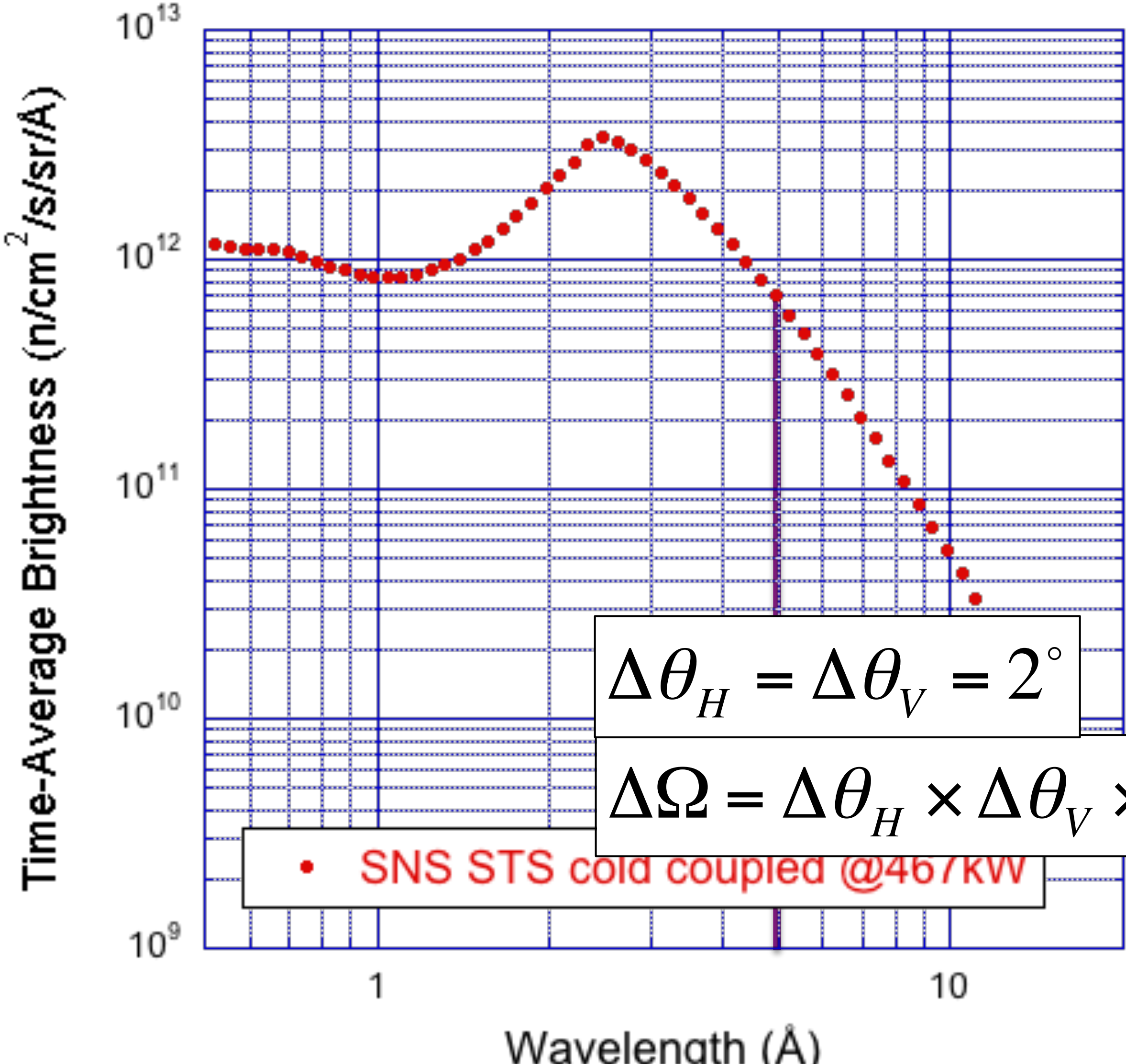
Example: SNS STS Cold Chopper Spectrometer



$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\,\mathrm{d}\lambda \times \Delta\Omega$$

$$\Delta\lambda = 1.6 \times 10^{-3}\,\text{Å}$$

$$\int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\,\mathrm{d}\lambda \text{ at } \lambda = 5\text{Å}$$

$$\approx 1.1 \times 10^{9}\ \text{n/cm}^2\text{/s/sr}$$

$$\Delta\theta_H = \Delta\theta_V = 2^\circ$$

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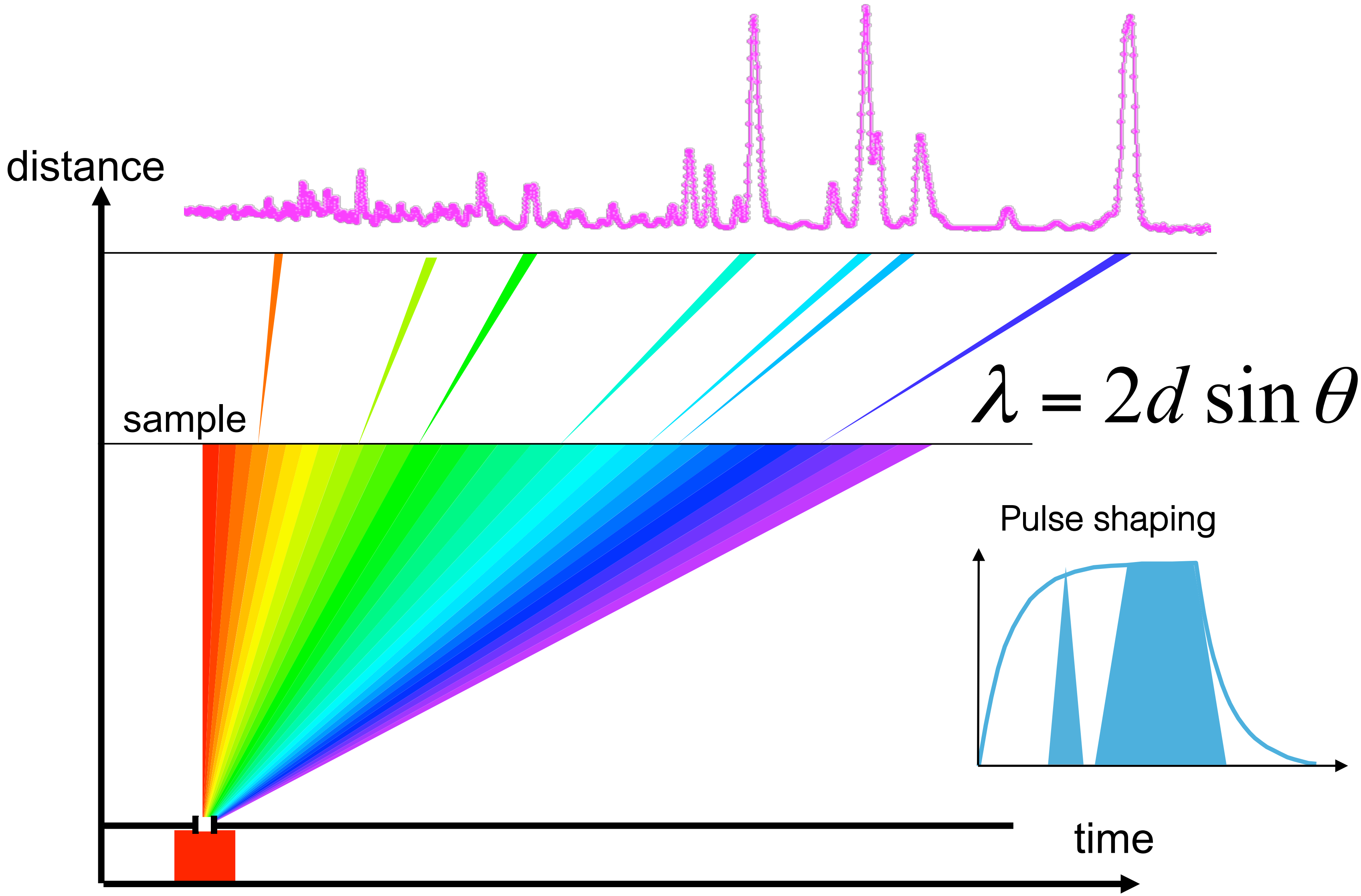
$$\Phi \approx 7 \times 10^{5}\ \text{n/cm}^2\text{/s}$$

Resolution Calculations

- Calculation of instrument parameters given resolution requirement
- Decide on the relevant quantity
- Express how it is calculated
- Calculate its uncertainty
  - requires the partial derivatives
- Match the various contributions
  - maximises flux for a given resolution

Example: ESS Powder Diffractometer



Example: ESS Powder Diffractometer

EUROPEAN SPALLATION SOURCE

$$d = \frac{\lambda}{2\sin\theta}$$

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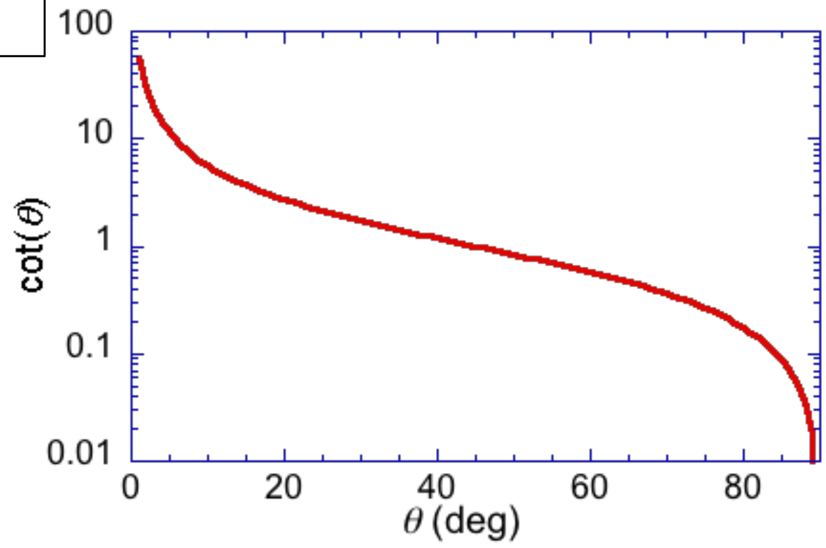

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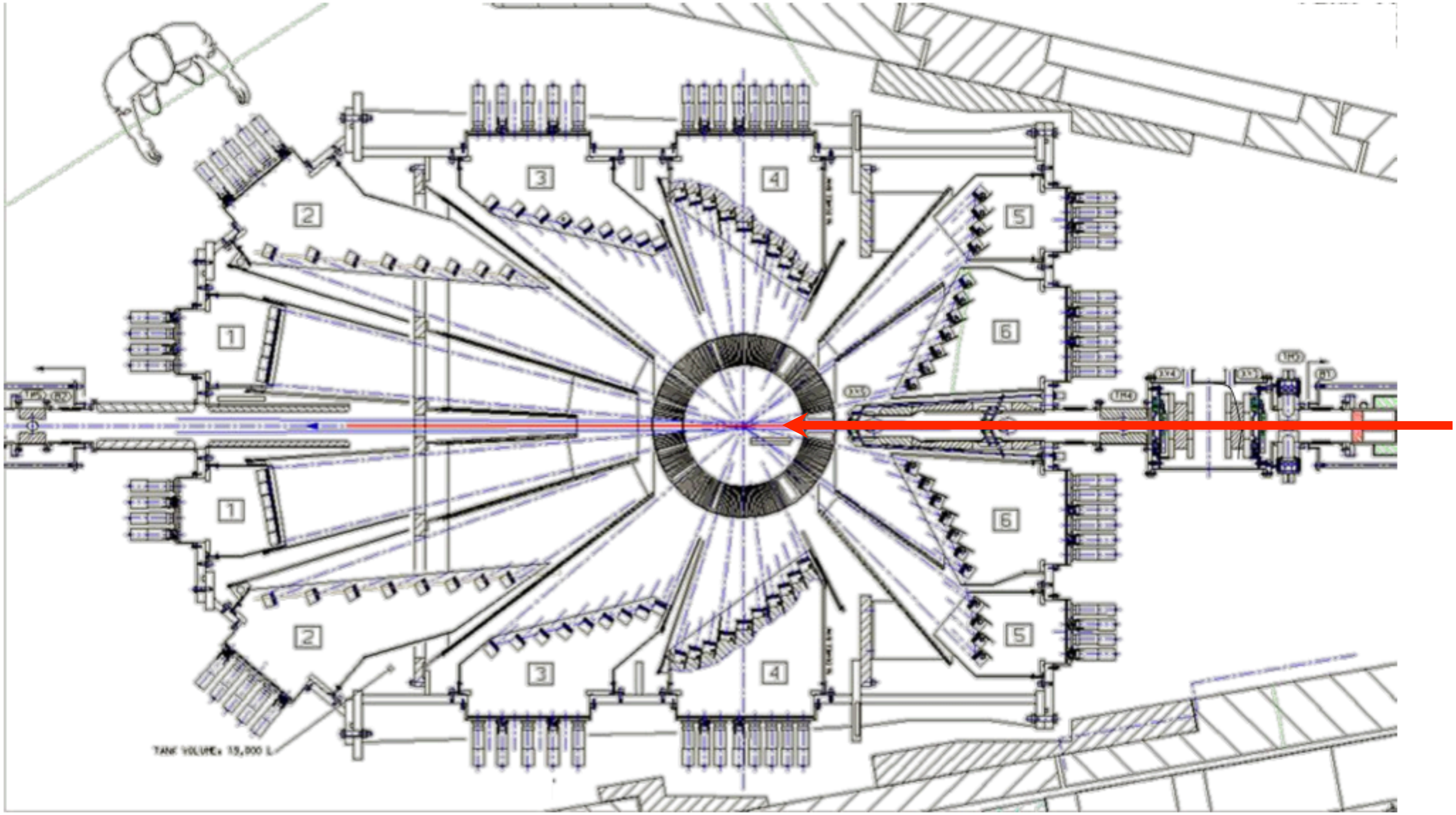

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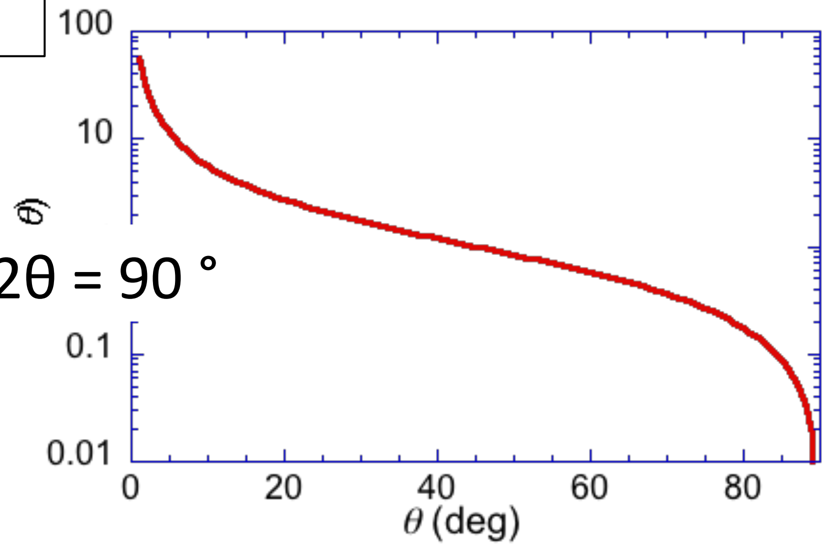
choose to match resolution terms for 2θ = 90 °



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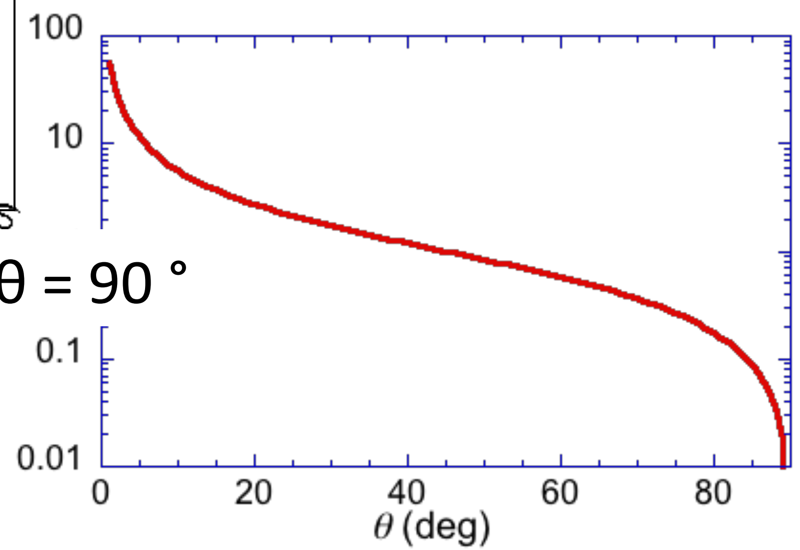

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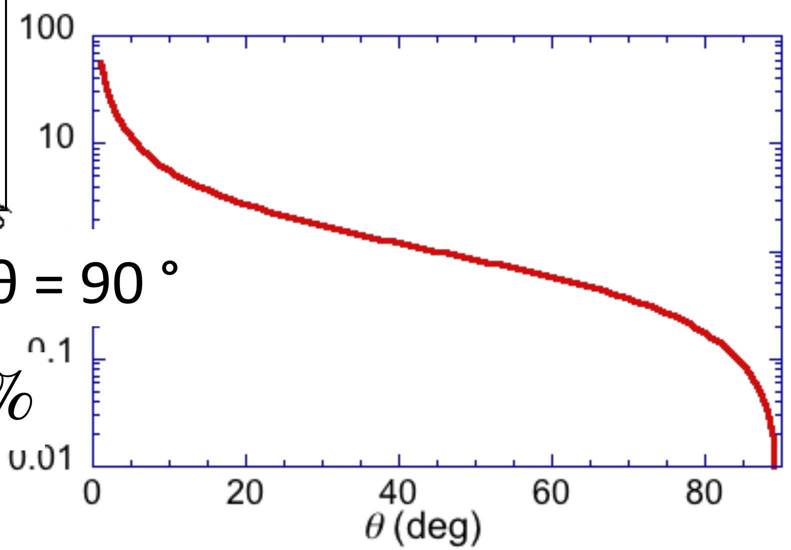

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science case: optimise for $\Delta d/d = 0.3\%$

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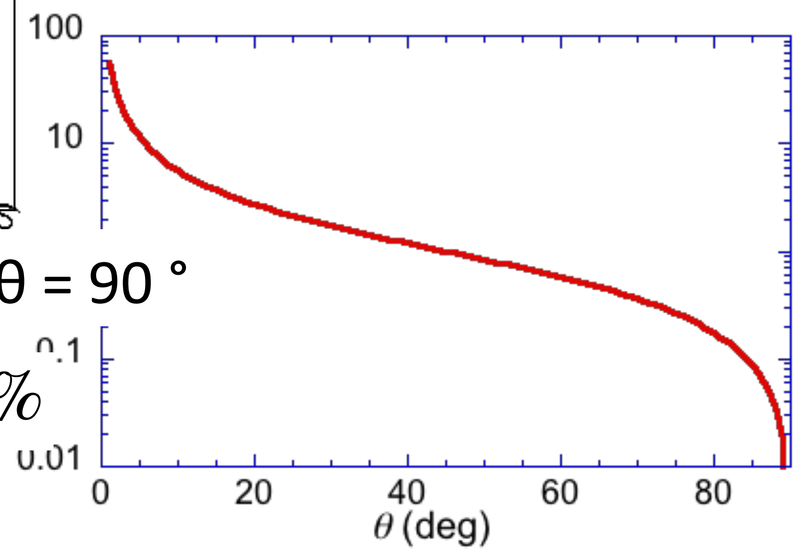


choose to match resolution terms for 2θ = 90 °

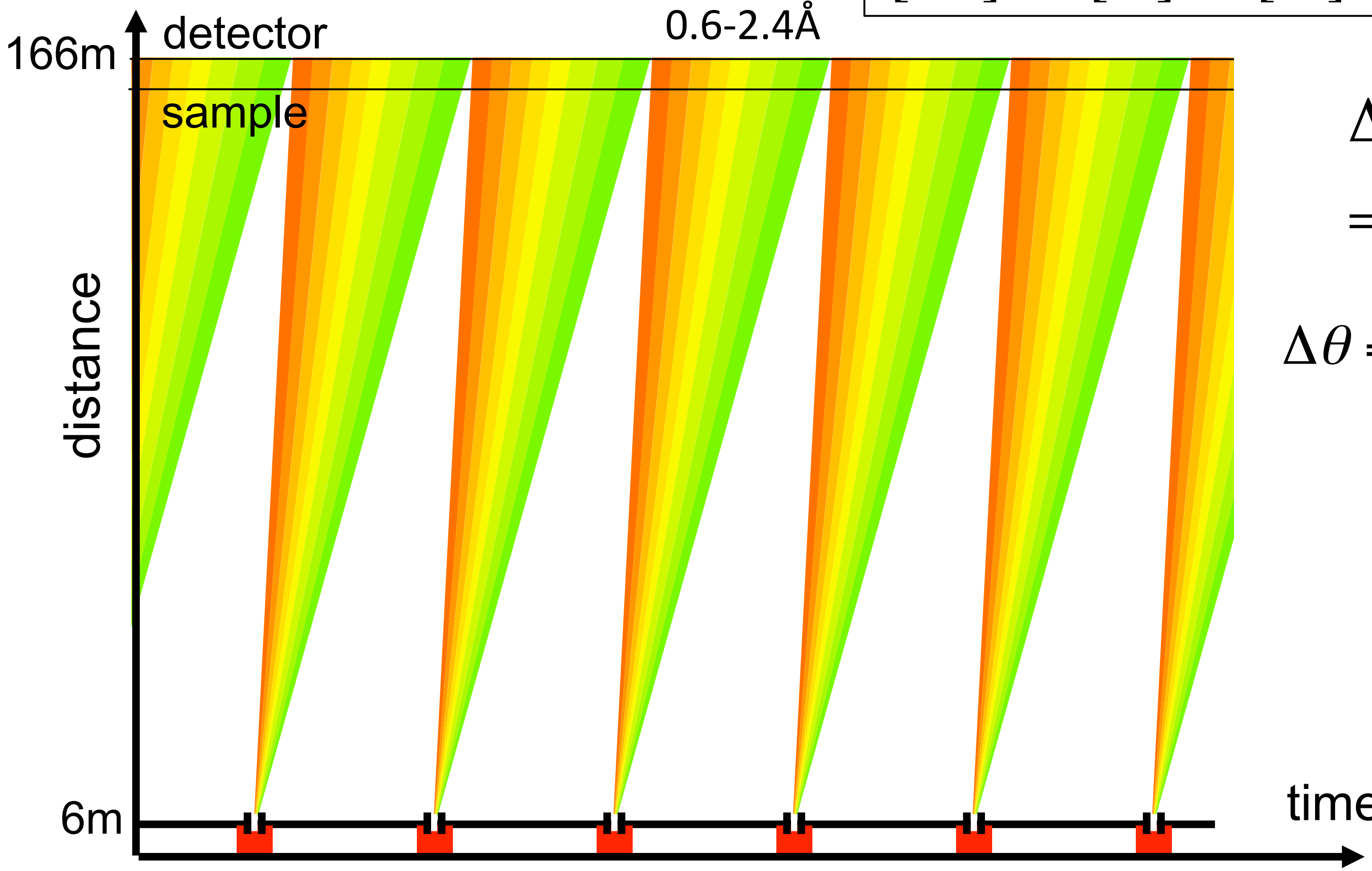
science case: optimise for $\Delta d/d = 0.3\%$

$$\Rightarrow \Delta t/t = 2\times10^{-3},\ \Delta\theta = 2\times10^{-3}$$

Example: ESS Powder Diffractometer

$$\lambda = 1.5\text{Å}, L = 160\text{m}$$

$$t[\text{ms}] = \lambda[\text{Å}] \times L[\text{m}] / 3.956 = 60.7\text{ms}$$



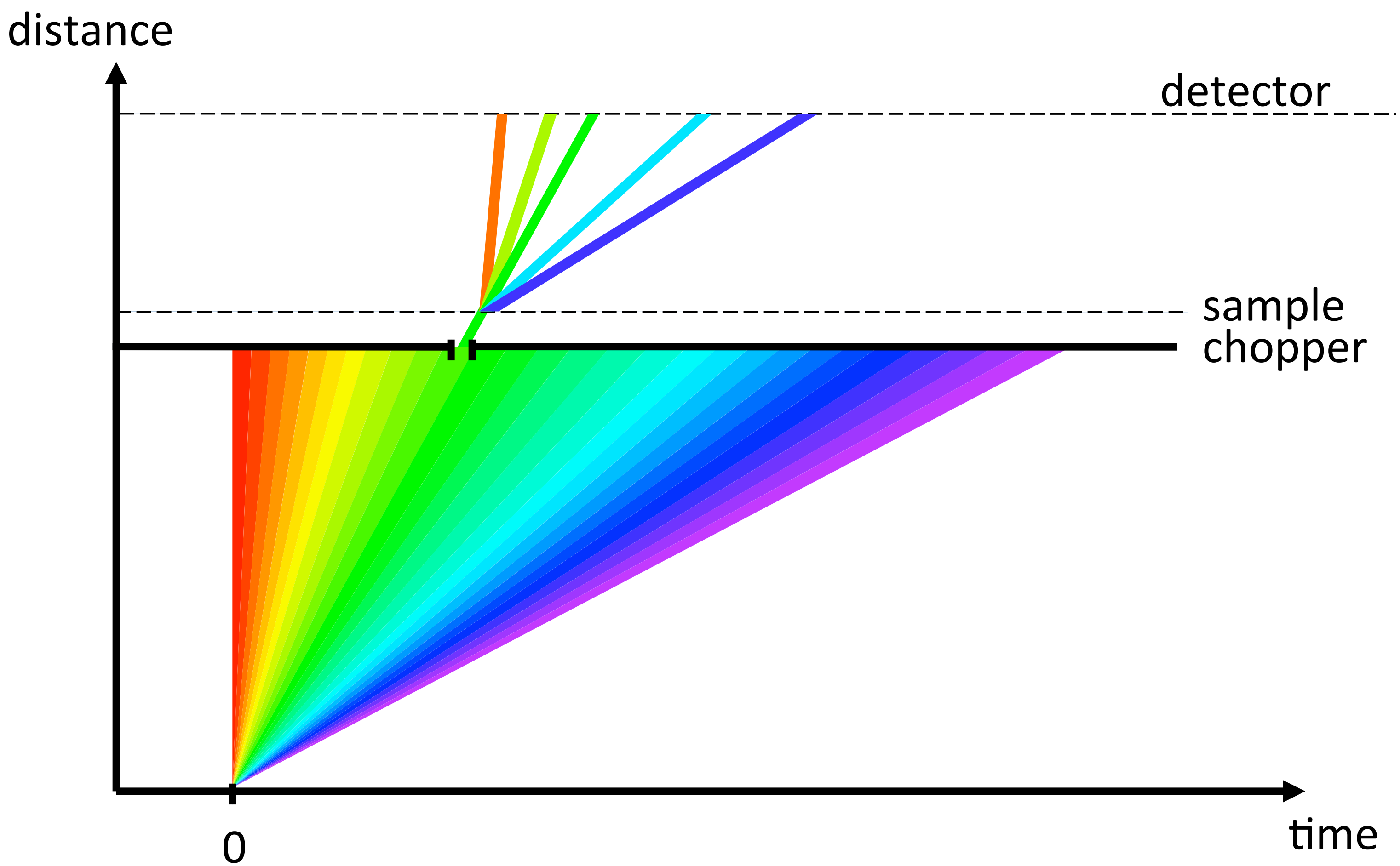
$$\Delta t / t = 2 \times 10^{-3}$$

$$\Rightarrow \Delta t = 120 \mu s$$

$$\Delta\theta = 2 \times 10^{-3} = 0.11^{\circ}$$

Example: SNS STS Cold Chopper Spectrometer

$$\hbar\omega = E_i - E_f$$



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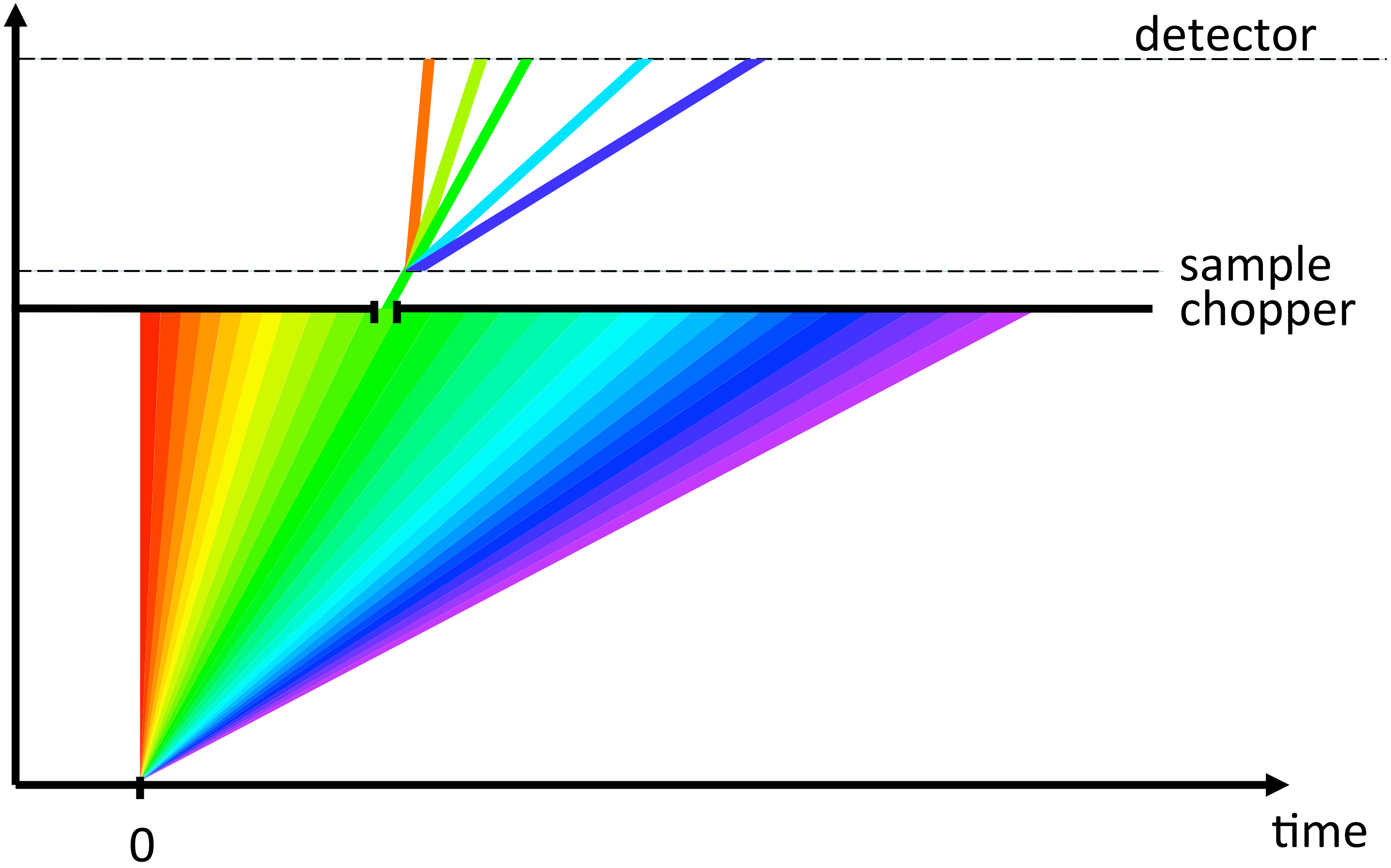
science case: "1% resolution at λ=5Å"



Example: SNS STS Cold Chopper Spectrometer

$$\hbar\omega = E_i - E_f$$

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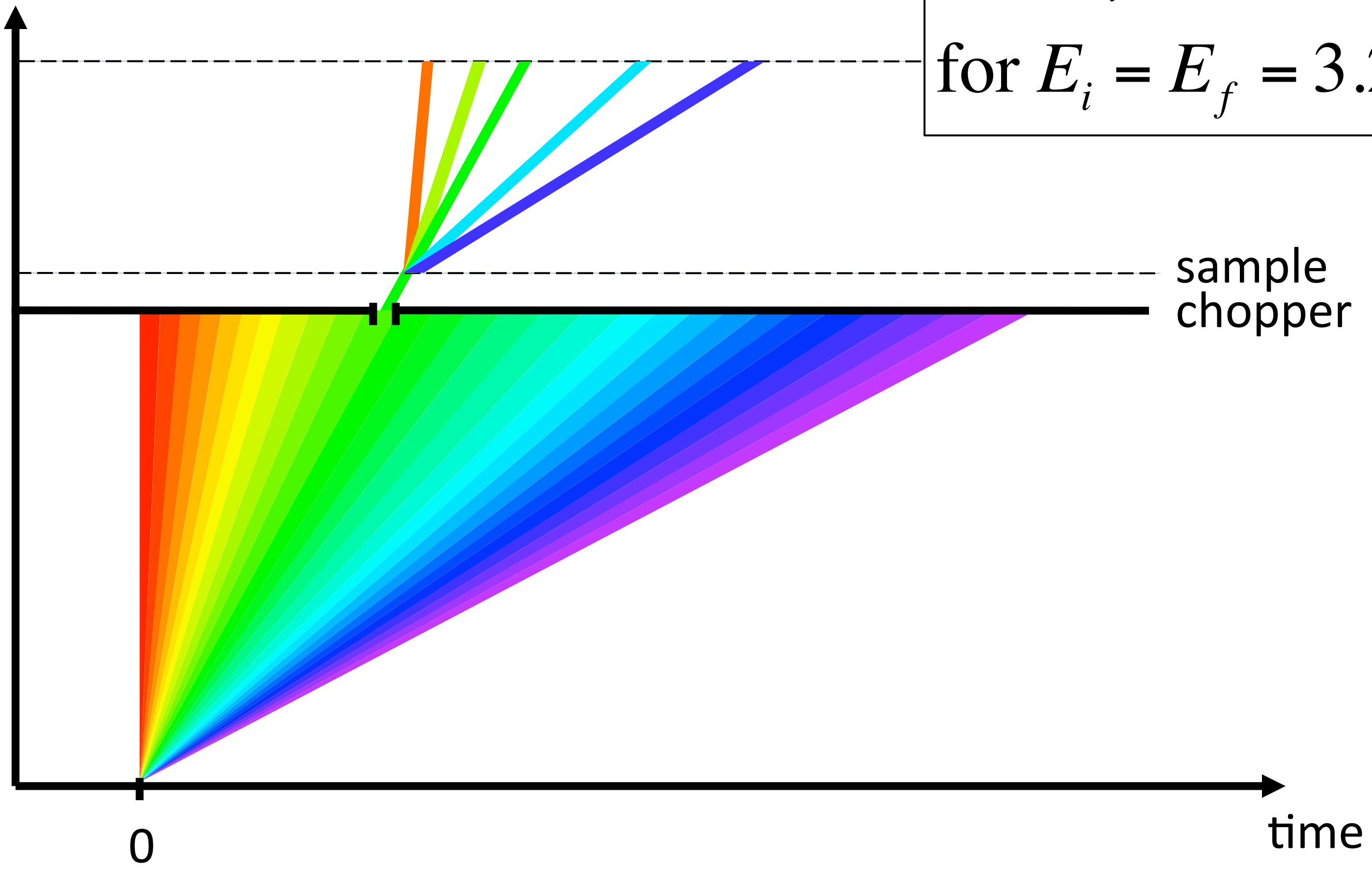
$$\Rightarrow \frac{\Delta\hbar\omega}{E_i} = 0.01$$

$$\text{for } E_i = E_f = 3.27\text{meV}$$



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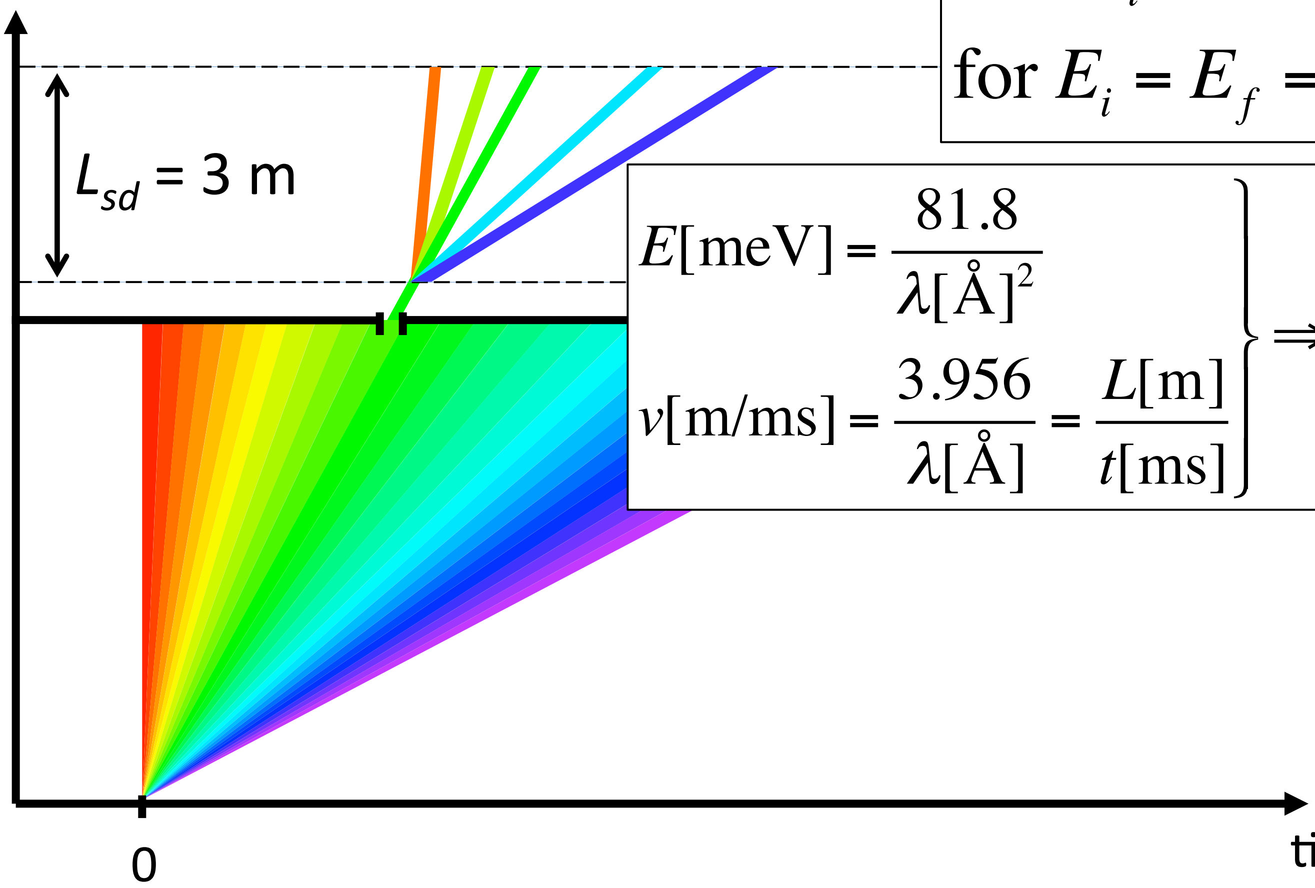

$$\left.\begin{array}{l} E[\text{meV}] = \dfrac{81.8}{\lambda[\text{Å}]^2} \\ v[\text{m/ms}] = \dfrac{3.956}{\lambda[\text{Å}]} = \dfrac{L[\text{m}]}{t[\text{ms}]} \end{array}\right\} \Rightarrow E = 5.227\frac{L^2}{t^2}$$

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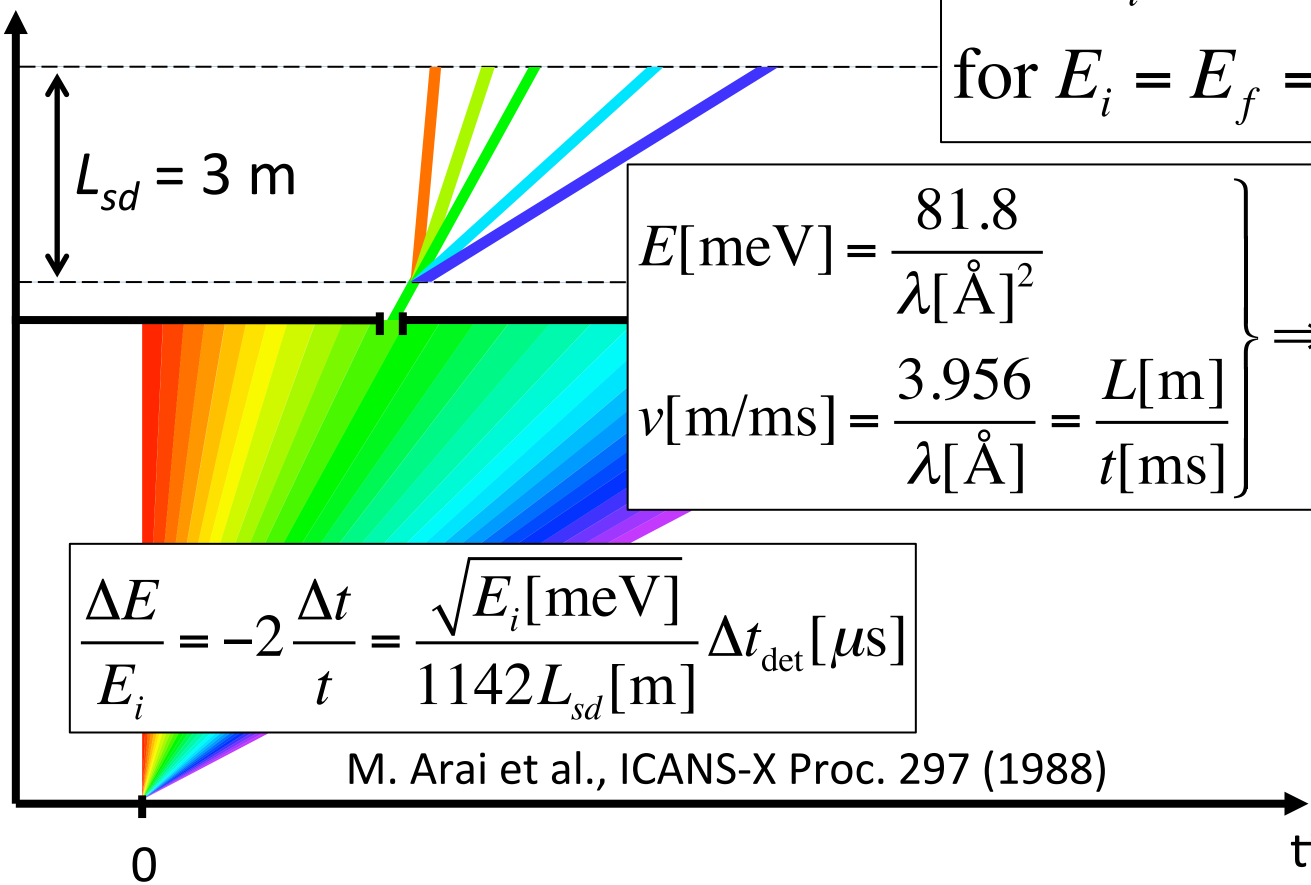

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$$\frac{\Delta E}{E_i} = -2\frac{\Delta t}{t} = \frac{\sqrt{E_i[\text{meV}]}}{1142 L_{sd}[\text{m}]}\Delta t_{\text{det}}[\mu\text{s}]$$

M. Arai et al., ICANS-X Proc. 297 (1988)

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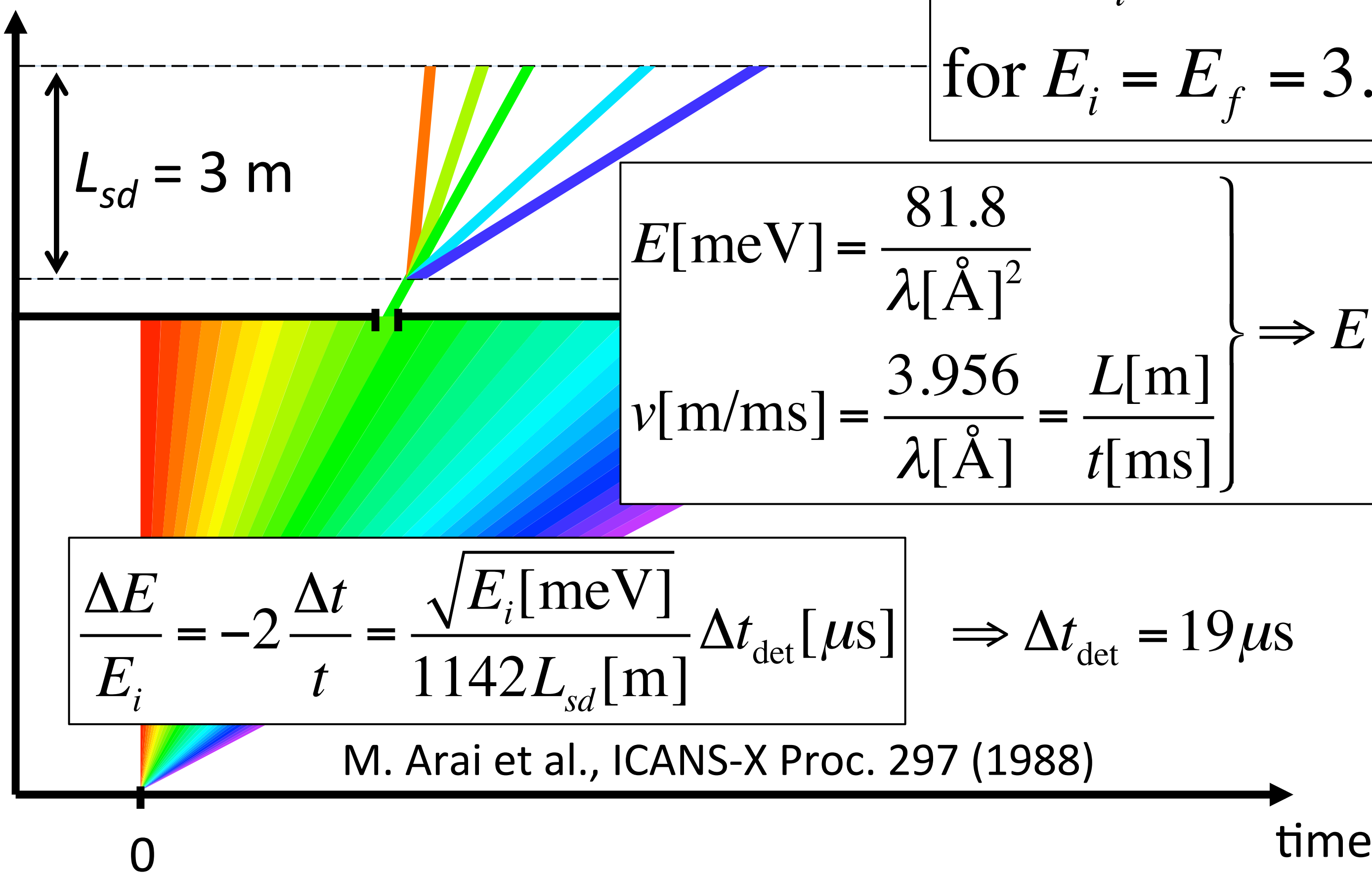

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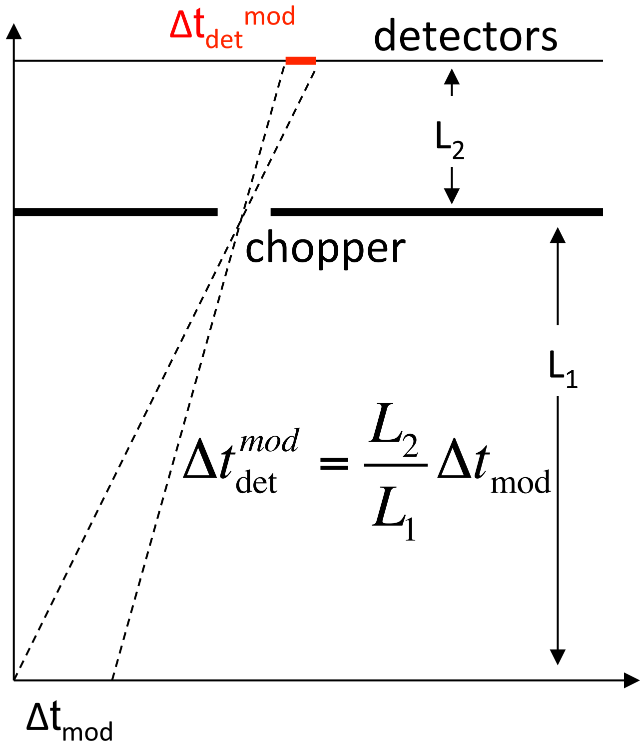
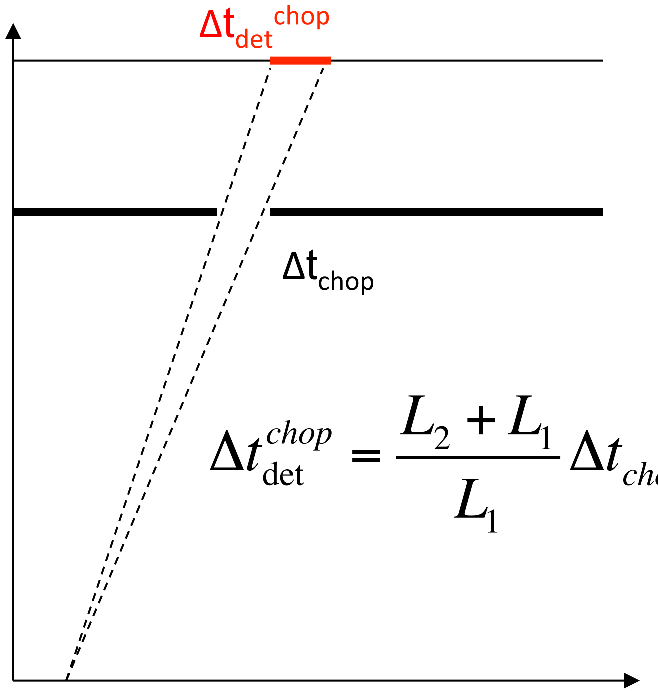
Example: SNS STS Cold Chopper Spectrometer

$$\Delta t_{\mathrm{det}} = \sqrt{(\Delta t_{\mathrm{det}}^{mod})^2 + (\Delta t_{\mathrm{det}}^{chop})^2}$$



$$\Delta t_{\mathrm{det}}^{mod} = \frac{L_2}{L_1} \Delta t_{\mathrm{mod}}$$

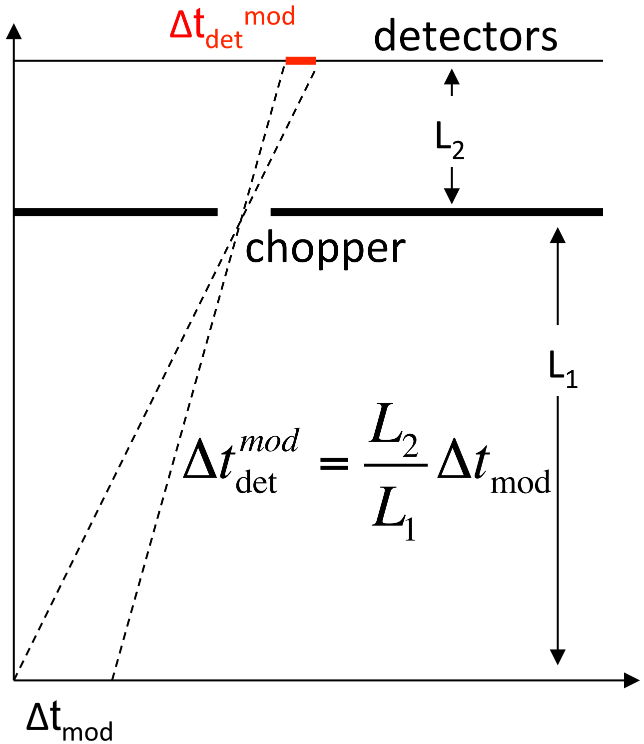


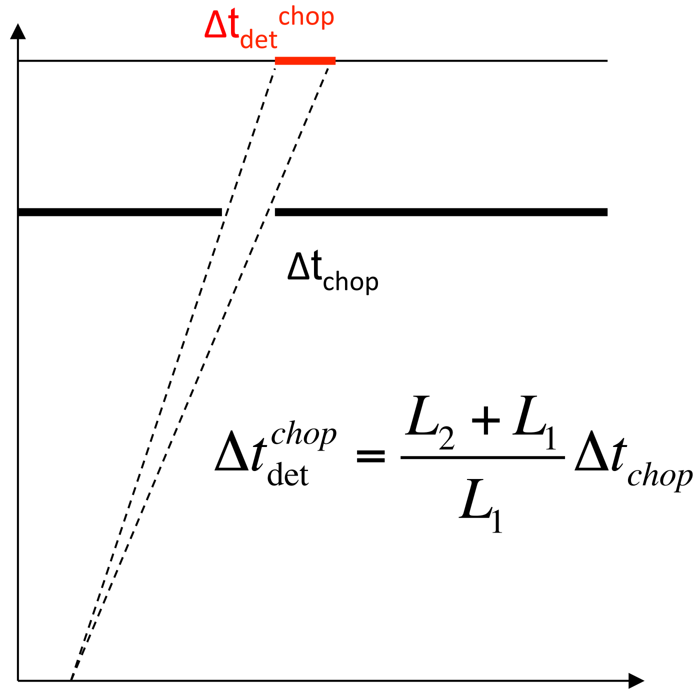
$$\Delta t_{\mathrm{det}}^{chop} = \frac{L_2 + L_1}{L_1} \Delta t_{chop}$$

Example: SNS STS Cold Chopper Spectrometer

$$\Delta t_{\det} = \sqrt{(\Delta t_{\det}^{mod})^2 + (\Delta t_{\det}^{chop})^2}$$

$$\Delta t_{\det}^{mod} = \Delta t_{\det}^{chop} = \frac{1}{\sqrt{2}} 19\mu s = 13.4\mu s$$





Example: SNS STS Cold Chopper Spectrometer

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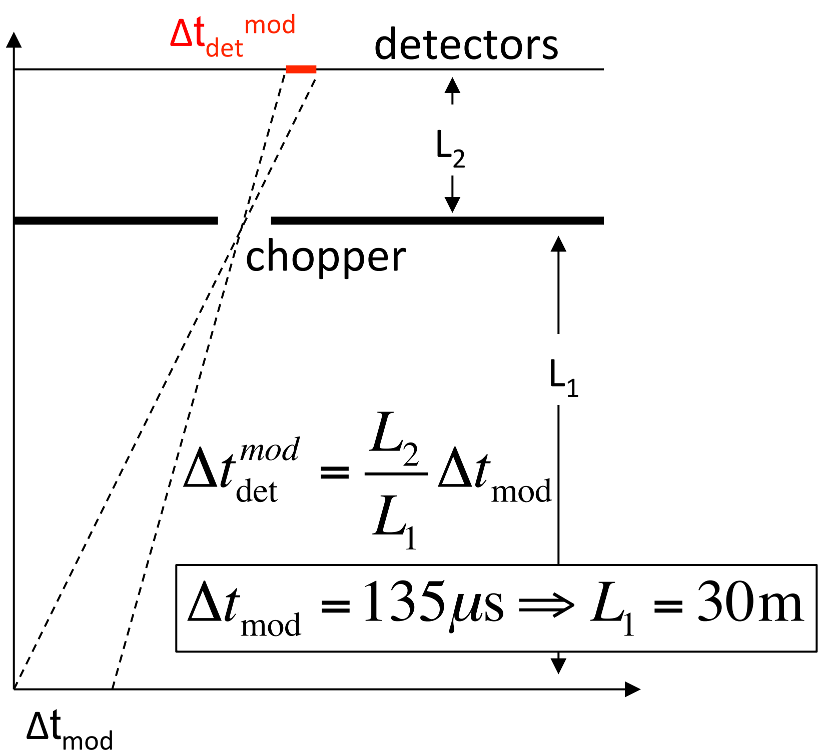

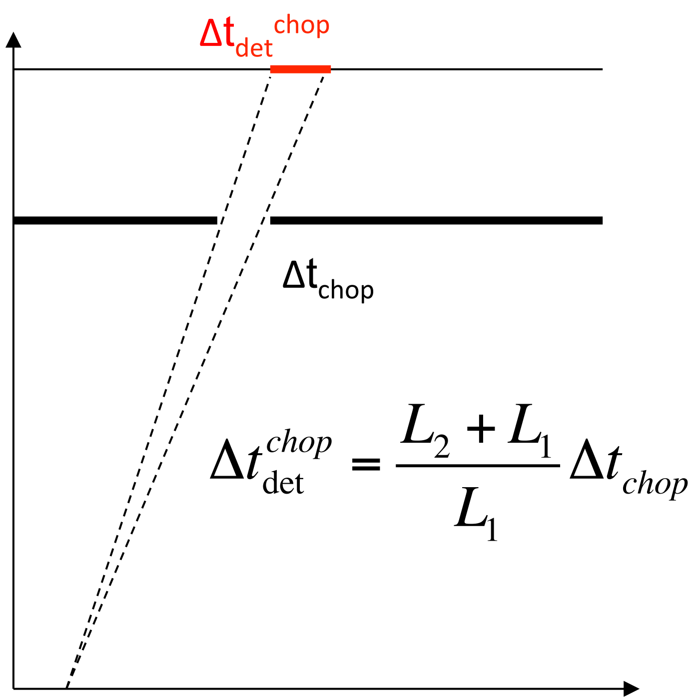

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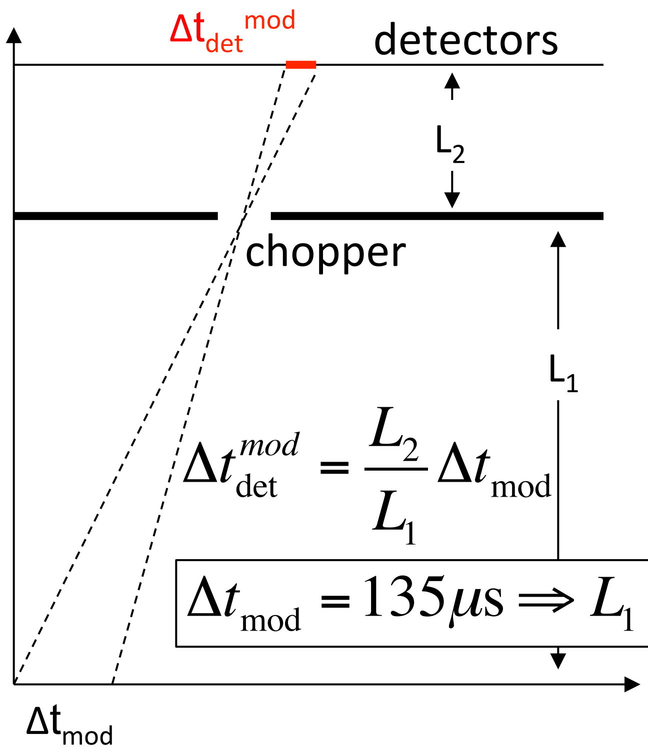
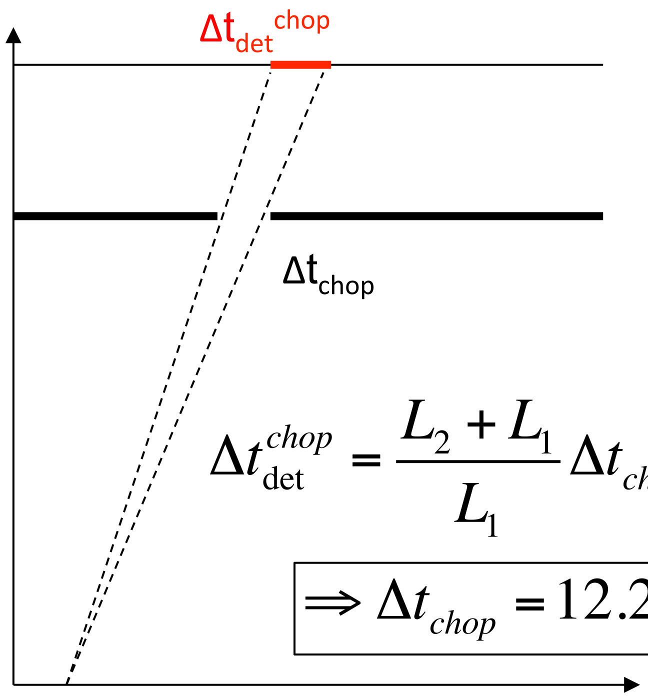


$$\Delta t_{\text{det}}^{mod} = \frac{L_2}{L_1} \Delta t_{\text{mod}}$$

$$\Delta t_{\text{mod}} = 135\mu s \Rightarrow L_1 = 30\text{m}$$



$$\Delta t_{\text{det}}^{chop} = \frac{L_2 + L_1}{L_1} \Delta t_{chop}$$

$$\Rightarrow \Delta t_{chop} = 12.2\mu s$$

Summary

- Peak vs Time-Average Brightness
- Brilliance Transfer
  - if you don't know it, set it 50%
  - very useful metric when evaluating simulations
- Calculation of flux given instrument parameters
- Flux at sample:

$$\Phi = \int_{\lambda_{\min}}^{\lambda_{\max}} B_{av}\,\mathrm{d}\lambda \times \Delta\Omega$$

- Resolution calculations
  - calculation of instrument parameters given resolution requirement
  - formulate the measurement requirement
  - calculate partial differentials
  - match resolution contributions
  - example: ESS powder diffractometer
  - example: SNS STS chopper spectrometer

Thank you!

EUROPEAN
SPALLATION
SOURCE

5th June 2015