Technical University of Denmark

Simulating neutrons - Moderation, extraction, shielding

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Publication date:
2014

Citation (APA):
Klinkby, E. B. (2014). Simulating neutrons - Moderation, extraction, shielding [Sound/Visual production (digital)]. Workshop on Neutron-Anti-Neutron Oscillations at ESS, Geneva, Switzerland, 12/06/2014

Simulating neutrons ::

Moderation, extraction, shielding

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Technical University of Denmark - Nutech

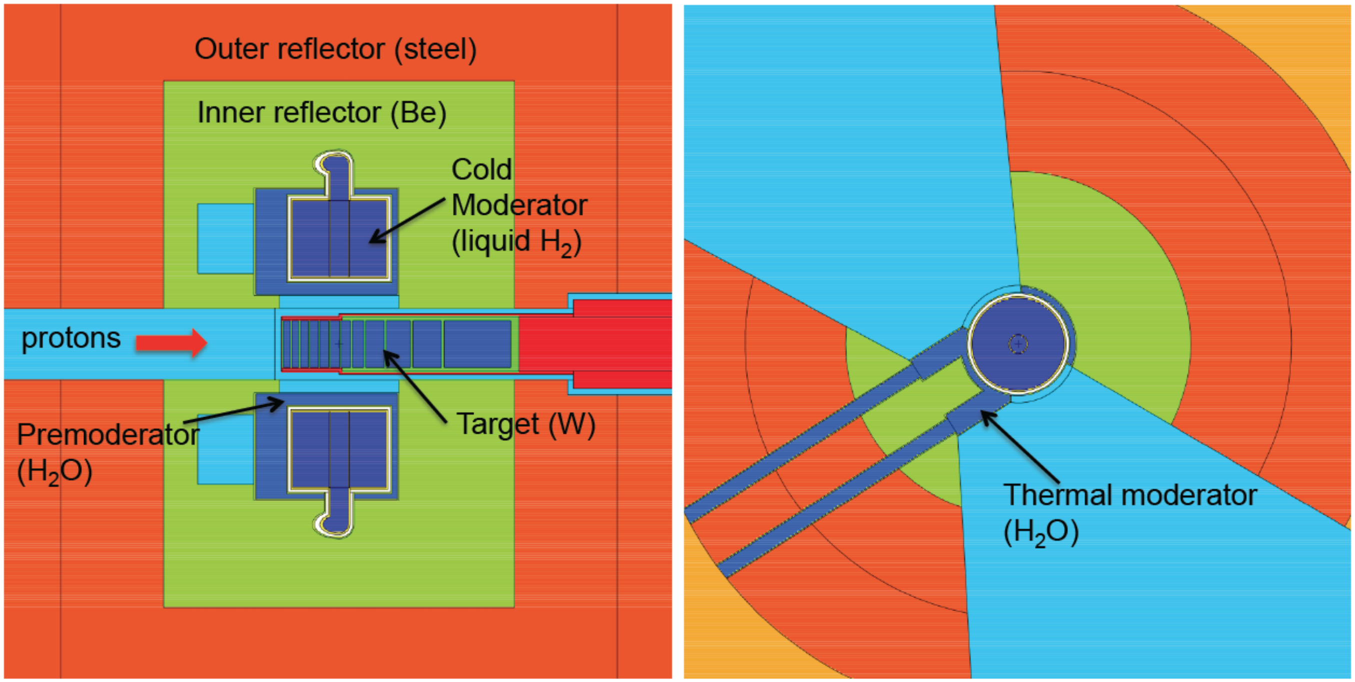
$n\bar{n}$ at ESS – CERN, June 12-13, 2014

www.europeanspallationsource.se

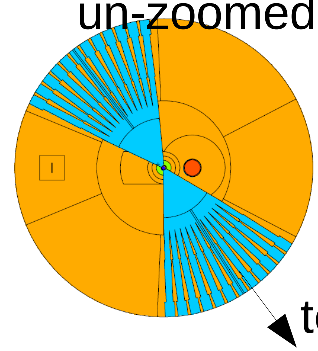
CONTENTS

- ❑ Cradle to grave:
  - Spallation
  - Moderation
  - Extraction
  - Backgrounds & Shielding
- ❑ Software interfaces
- ❑ Possible configurations

TDR configuration :: 2 tall moderators



- Neutrons extracted through window at 2m
- Instrument separation: 5° (=> 17.5 cm at 2m)
- Guides should bend to avoid streaming of fast neutrons

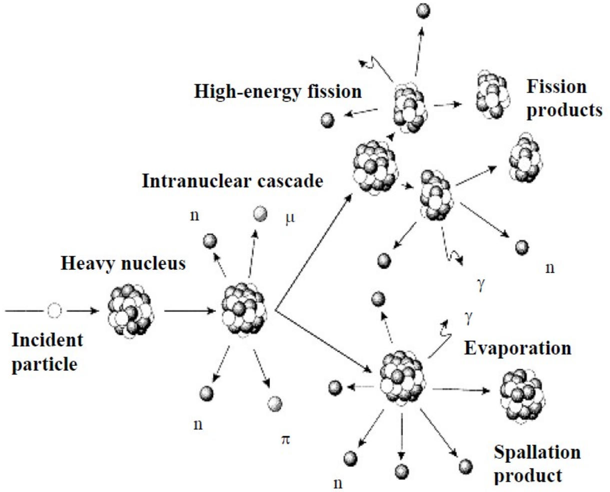


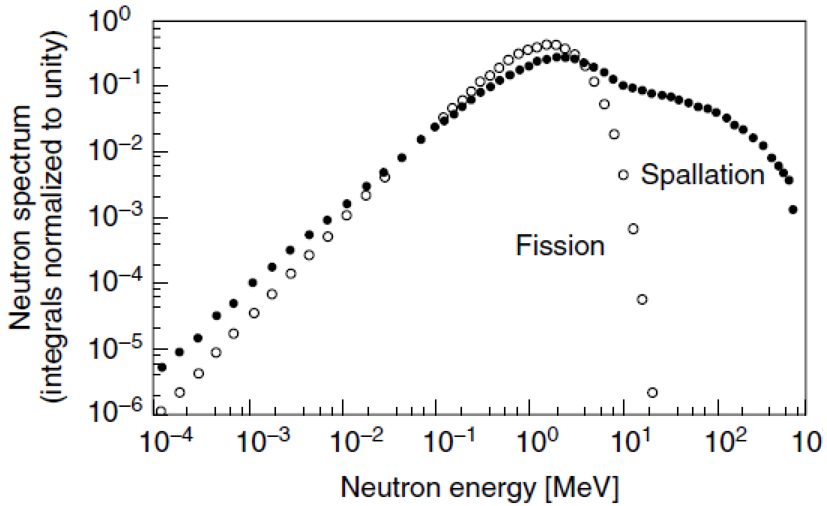
Neutron creation:: spallation

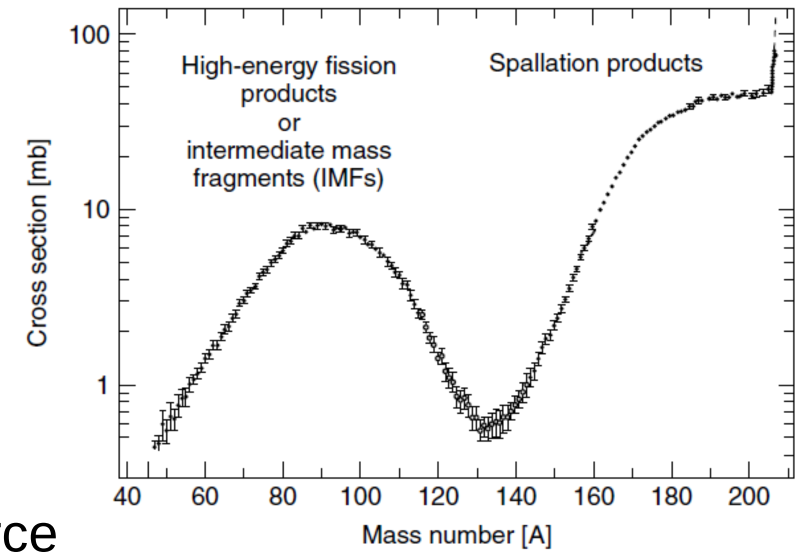
- Proton de Broglie wavelength:
- $\lambda = hc / (2m_p c^2 E_p)^{½} = 6\cdot10^{-16}$ m

Size of nuclei: ~10^{-14} m

- ⇒ protons interact with nucleons not nuclei
- Spallation is efficient: ~70 neutrons pr proton at 2GeV
- Theoretically complicated: software use models







Alternatively: use reactors: Continuous source

Neutron moderation :: from MeV to meV

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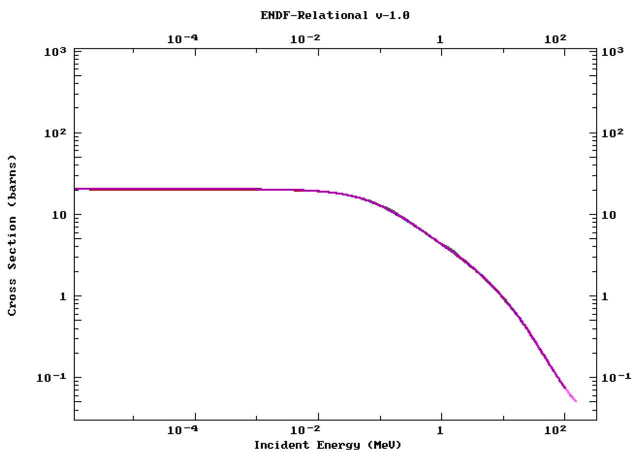
- Scattering instruments probe distances: ~Å $=10^{-10}$ m $\Rightarrow$ neutrons most be cooled to meV.

- n,H cross-section is large → Water is efficient for thermalization. A few cm is sufficient

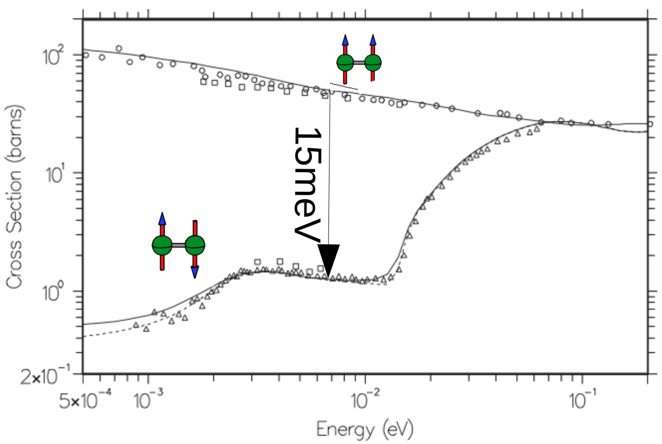
- 20K Para-hydrogen (spin flip scattering) is used.
- ~1cm is sufficient

- Para-hydrogen ~transparent for cold neutrons

- Simulation wise, the interactions of protons with the target, neutron creation and moderation is modeled using *MCNP*



n,H cross-sections



MCNPX :: Monte Carlo N-Particle Transport Code

EUROPEAN SPALLATION SOURCE

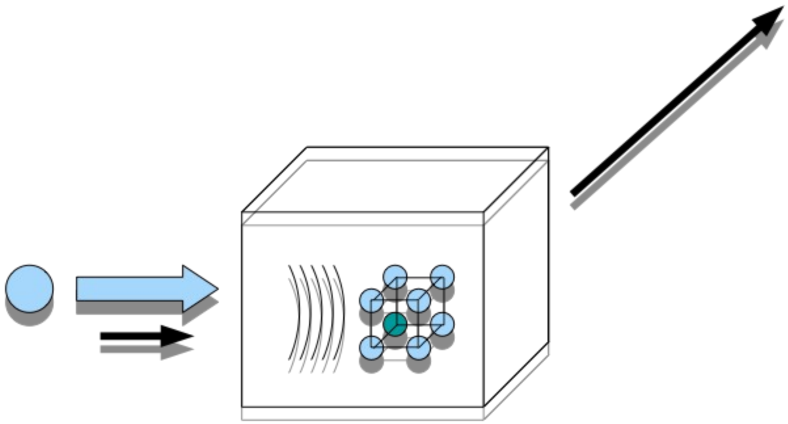
- Standard MC code for neutron physics (spallation sources, reactors, weapons...)
- Use Evaluated Nuclear Data – ENDF-VII
- Use INCL, Bertini, Isabel or CEM
- Limitations:
  →Most applications based on free gas model. Coherent scattering only accurate for powders.
  →Must be supplemented with scattering kernels for accurate description of processes at low energy (eV range)
  →Slow
  →Licensing: distribution is restricted, personal license required

History box

- During WW2, "numerical experiments" were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.
- Notable fathers:Neuman,Ulam Metropolis
- Named "Monte Carlo" after Ulam's fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially "implemented" by letting large numbers of women use tabularized random numbers and hand calculators for individual particle calculations
- Later, analogue and digital computing devices were used

Ray tracing techniques

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation whenever possible
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved- I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



<u>Numerous codes exist:</u>

- *NISP*
- *IDEAS*
- *Instrument Builder*
- *McVine*
- *RESTRAX/SIMRES*
- *VITESS*
- *McStas,*
- *NADS*
- *PHITS*
- *NTRANS*

- Result: A realistic and CPU-time efficient transport of neutrons in the thermal and cold range

Getting neutrons from A to B

- *Ni* and *Ti*: chemically similar, but different refraction indices

⇒ Coating with alternating layers: “Supermirrors”

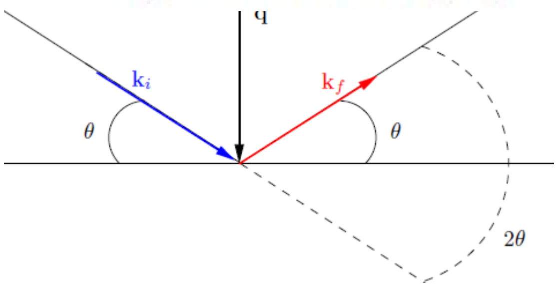
⇒ Neutron guides

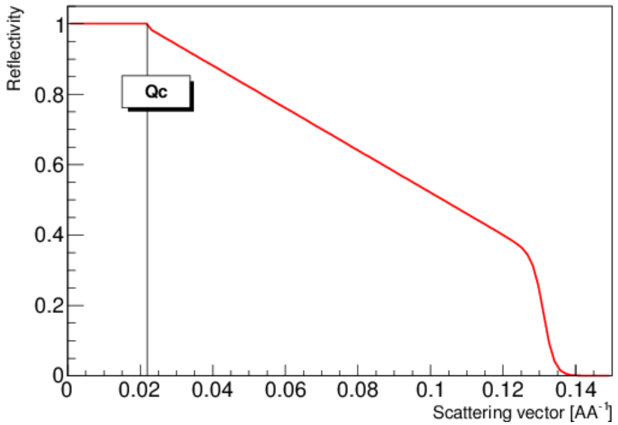
⇒ Transport cold/thermal neutrons (~without loss) to radiation safe distances

⇒ Energy measurement by TimeOfFlight.

All of this +*choppers, velocity selectors, collimators, monocrometers etc* is simulated in eg *McStas*

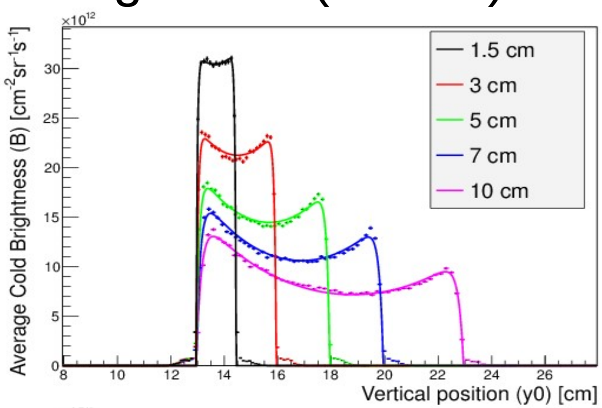
$$q = 2k\sin(\theta)$$

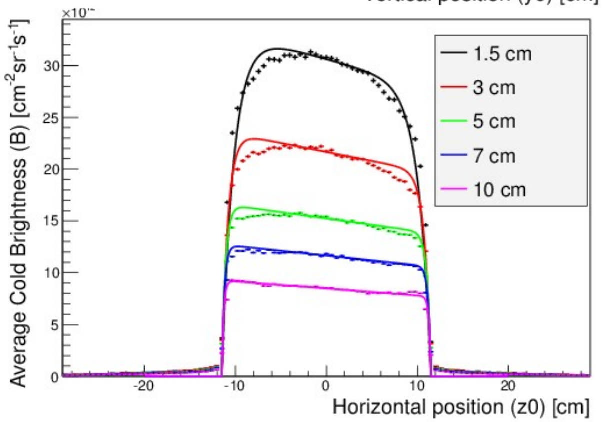


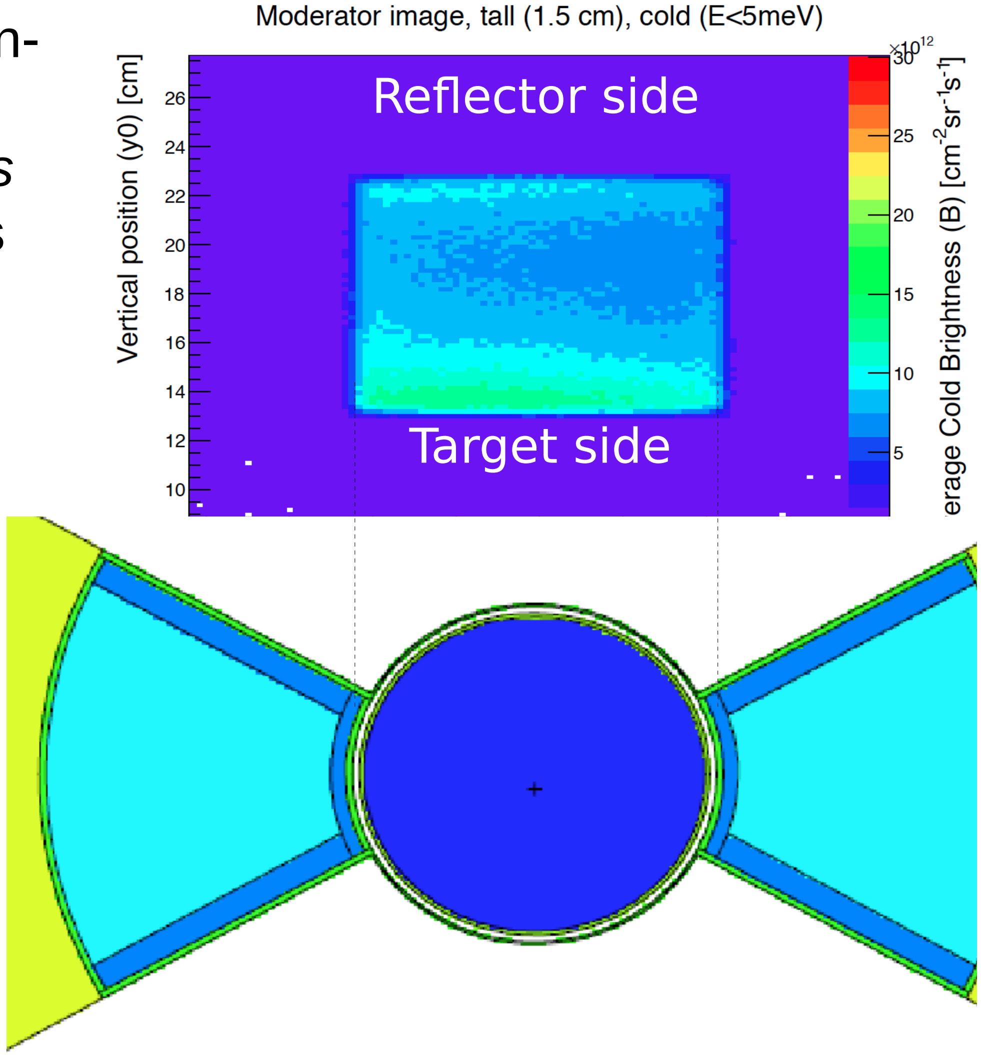


Instrument optimizations :: cold source

- Important to take into account non-uniformities.
- Source is parametrized in *McStas* using below (*MCNP*) distributions

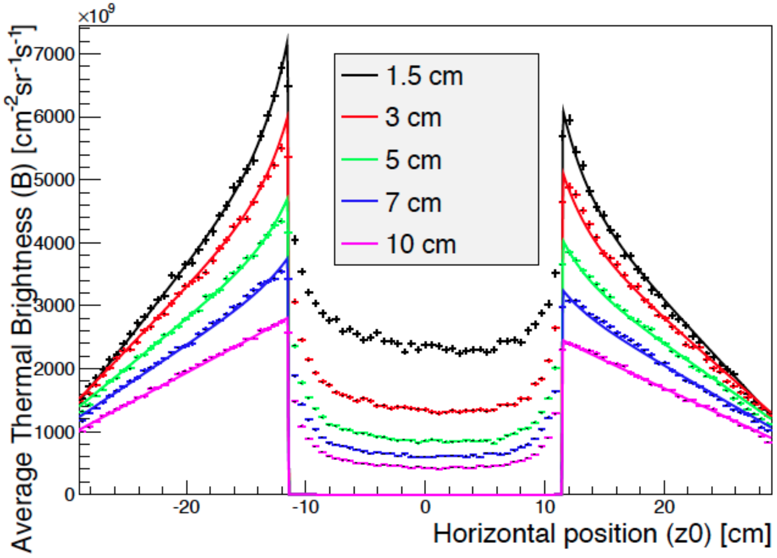


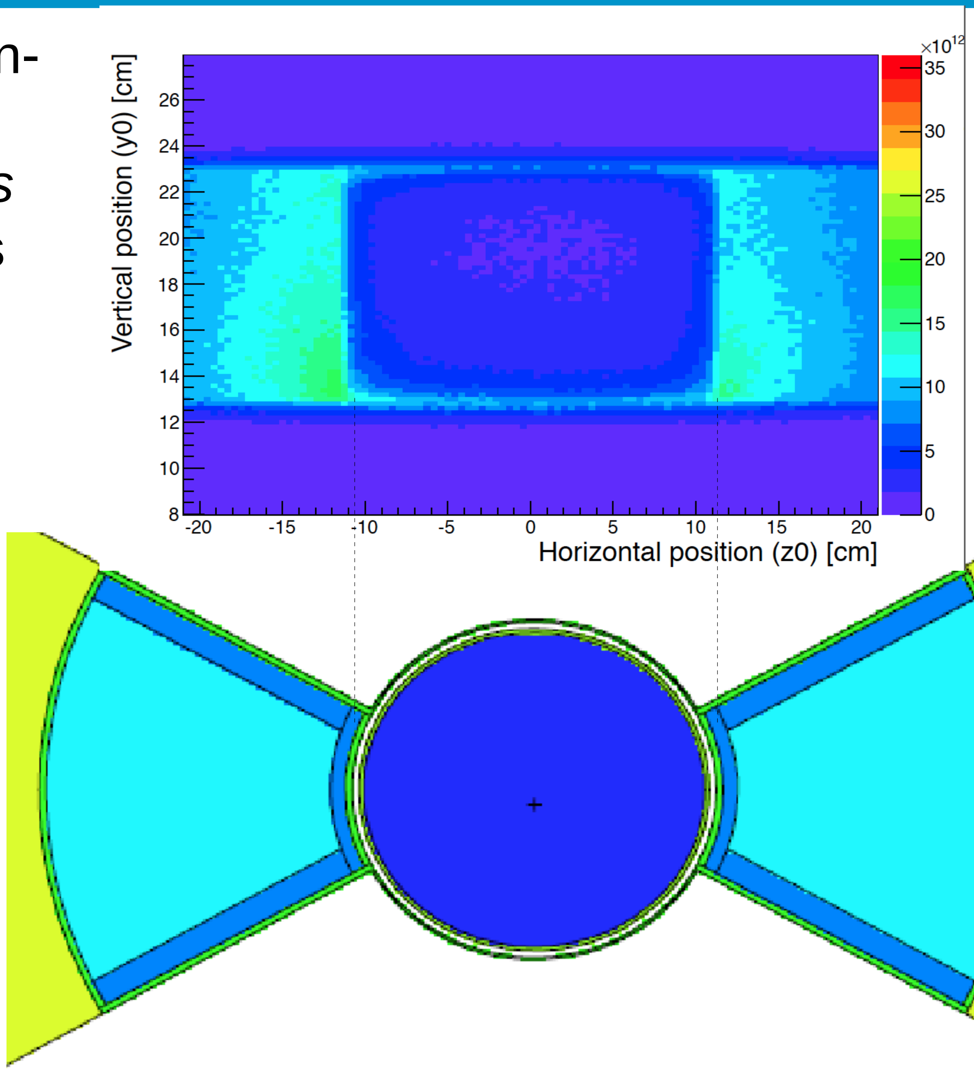




Instrument optimizations :: thermal source

- Important to take into account non-uniformities.
- Source is parametrized in *McStas* using below (*MCNP*) distributions

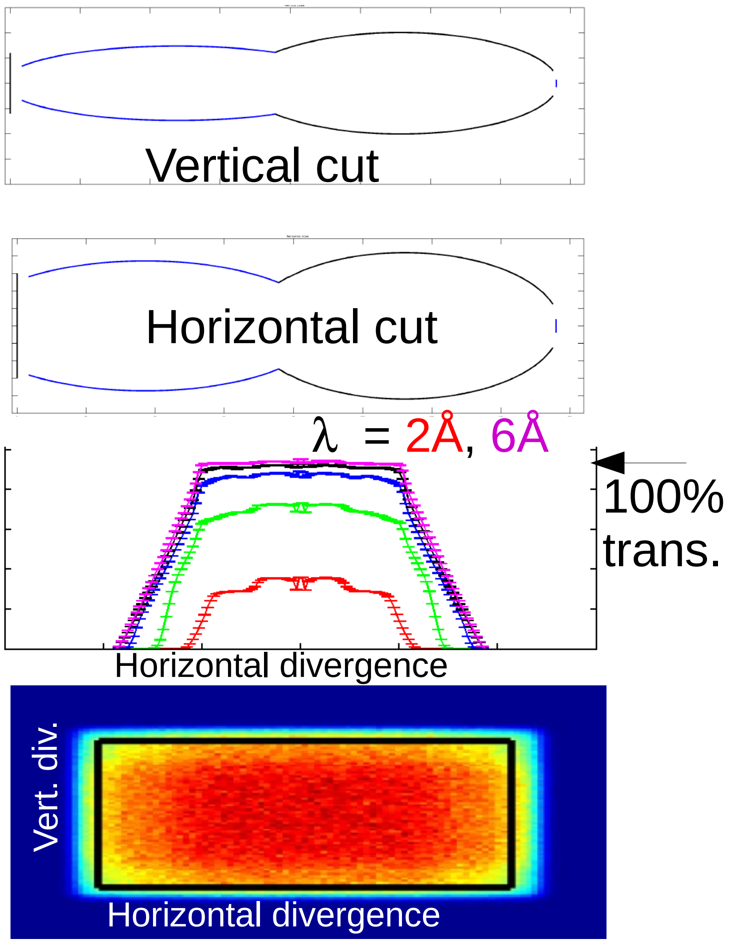




Instrument optimizations :: guide

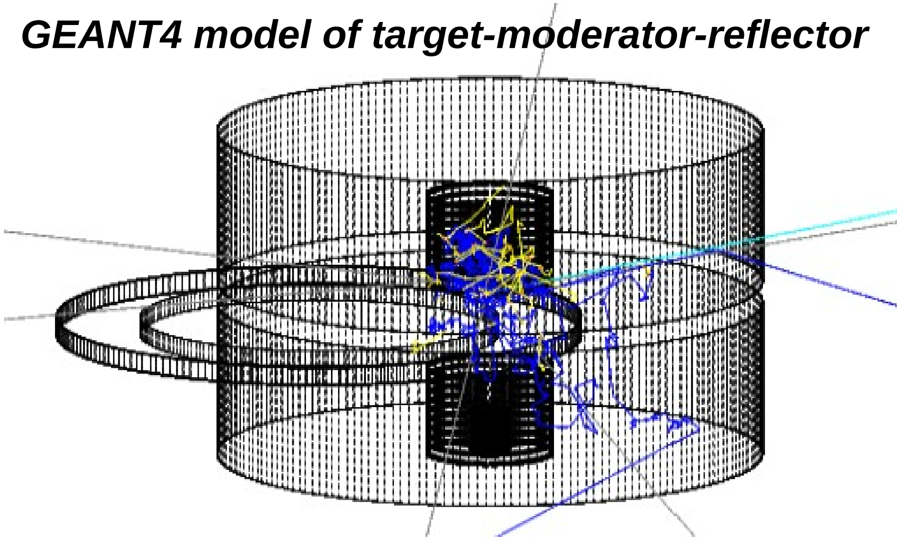
- Phase-space for instrument optimization is huge
- To ease the task, one additional of layer of software is added on top of *McStas: guide_bot*
- Given a user-selected set of *components* and allowed *parameters, dimensions* etc, *guide_bot* uses a Swarm algorithm to find the guide which best transfer the beam from the beam extraction to the sample
- Example: elliptical-elliptical, ...

Example of guide_bot output



Shielding and backgrounds

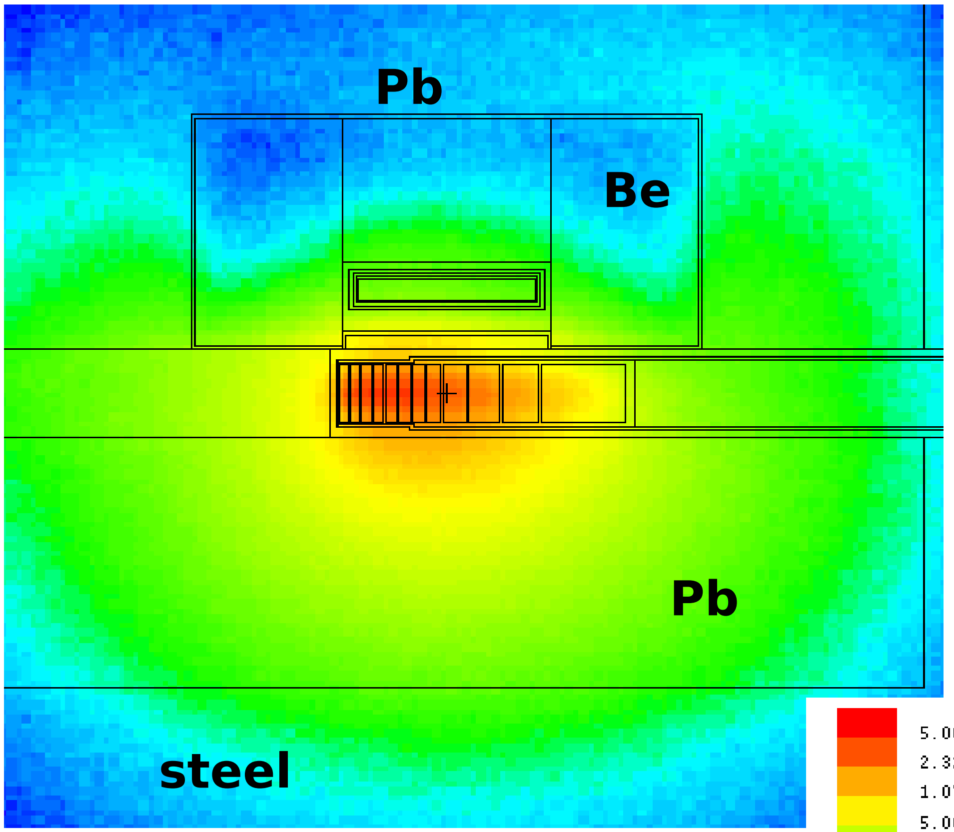
GEANT4 model of target-moderator-reflector

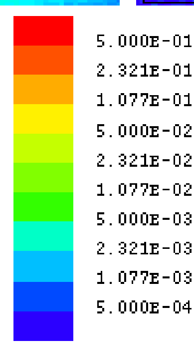


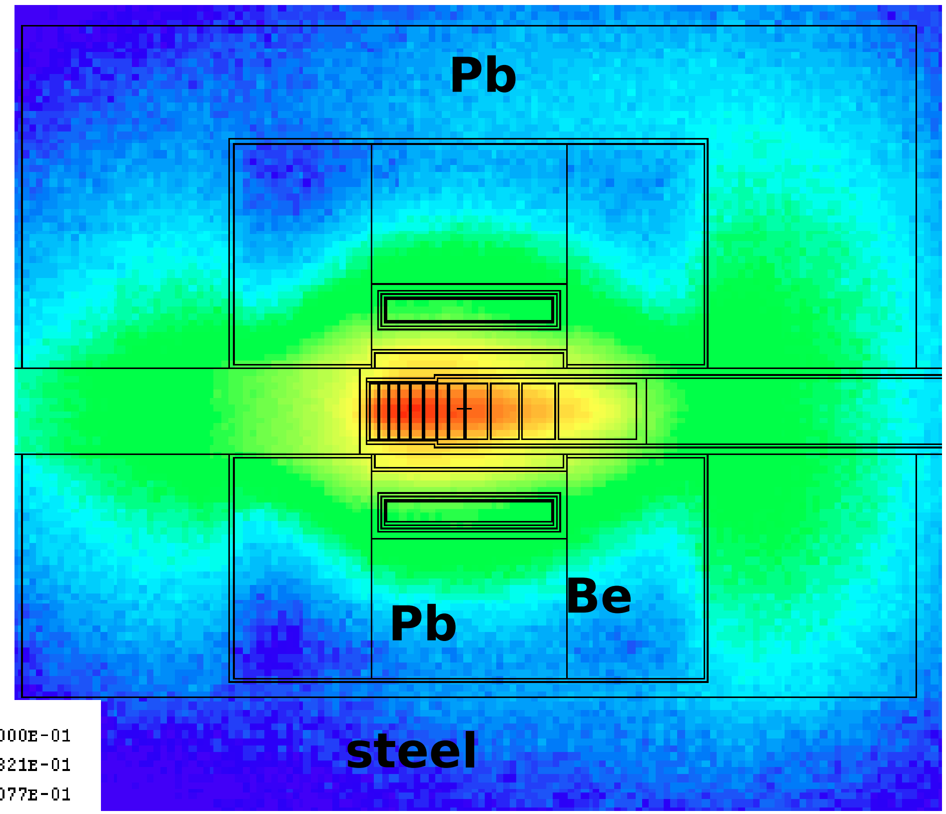
- In addition to cold/thermal neutrons, sample and detectors are subject to backgrounds (n, π, γ, p, from the spallation hotspot + secondaries).
- Not naturally incorporated in ray-tracing codes
- Ongoing efforts to mirror the *MCNP* model of target, moderators, reflectors and beam extraction in *GEANT4* (used for detector simulations).

Shielding and backgrounds :: Fast neutrons

EUROPEAN SPALLATION SOURCE





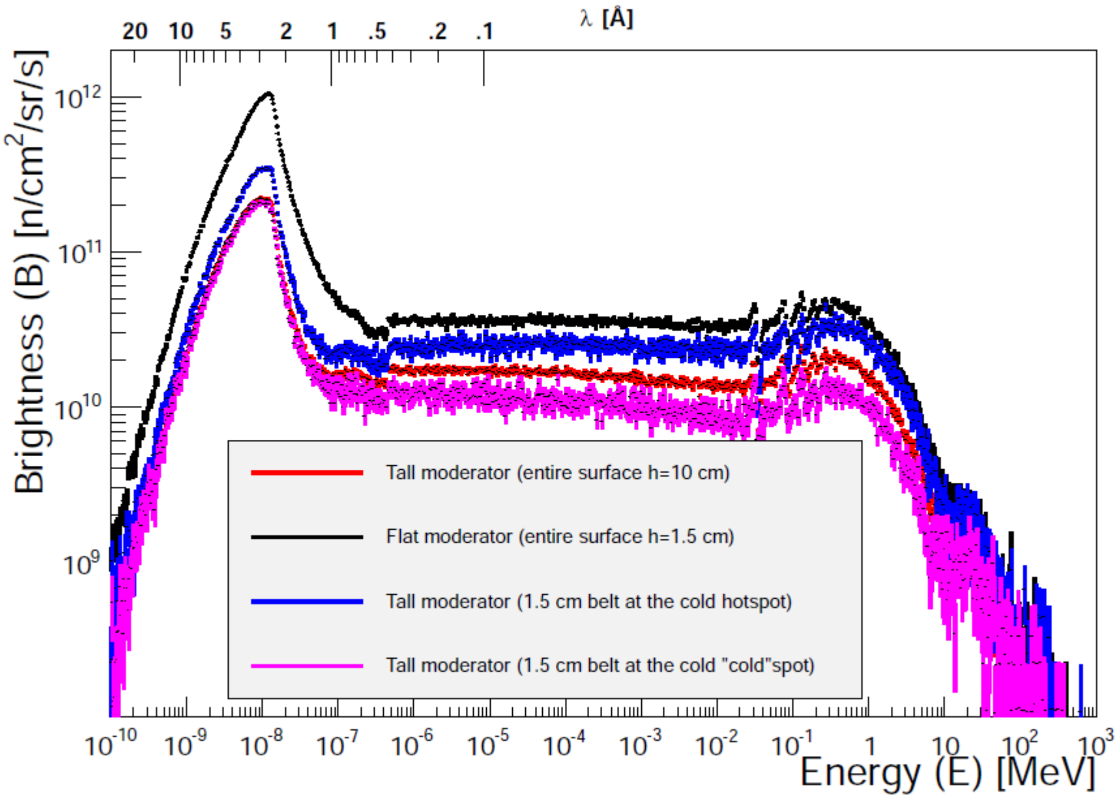


Reflector material choice,
impacts shielding requirements

n/cm²/primary proton
***E*>0.1 MeV**

Shielding and backgrounds

Neutron spectrum at beam extraction (radii=2m)

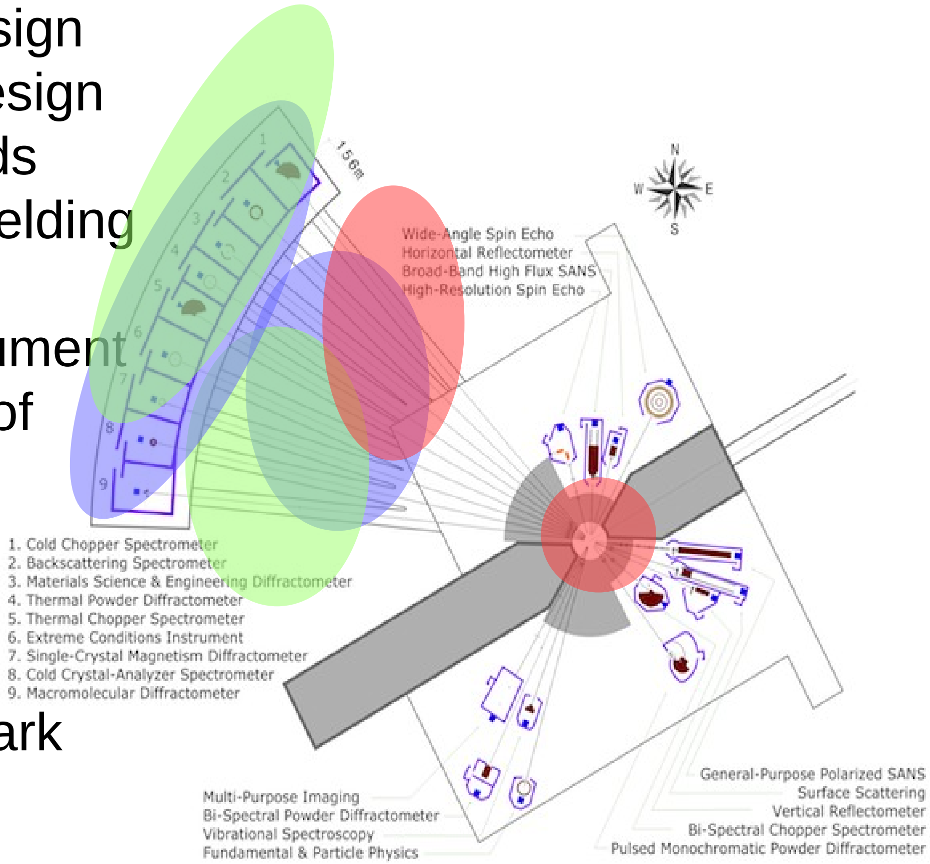


- To estimate shielding and background, individual neutron states are handed from *MCNP* to a *ROOT* based analysis framework.
- Avoids inaccuracies from integration

Monte Carlo vs. ray tracing – where are we heading?

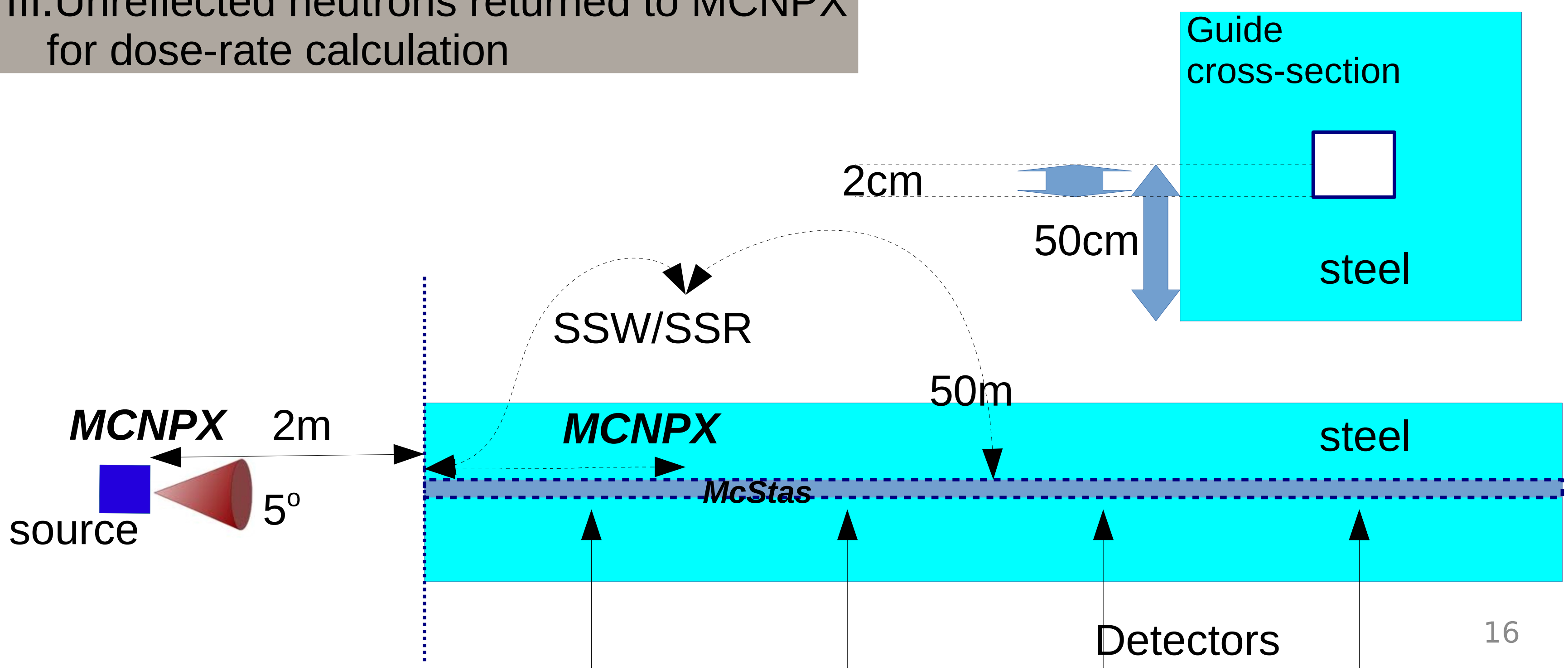
- *MCNP:* target, moderator, reflector design
- *McStas* (+*guide_bot*) for instrument design
- *GEANT4* for shielding and backgrounds
- Vitess & NADS & Particle swarms: shielding & optics
  - design documentation for the instrument
- *MCNP*: safety, dose-rates (future use of FLUKA or MARS)
- *GEANT4:* detector design

- ⇒ Interfacing is important.
- Efforts ongoing to merge and benchmark



Example :: MCNP-McStas interface

I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface
III. Unreflected neutrons returned to MCNPX for dose-rate calculation



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Example :: MCNP-McStas interface

I. Neutrons generated with MCNPX
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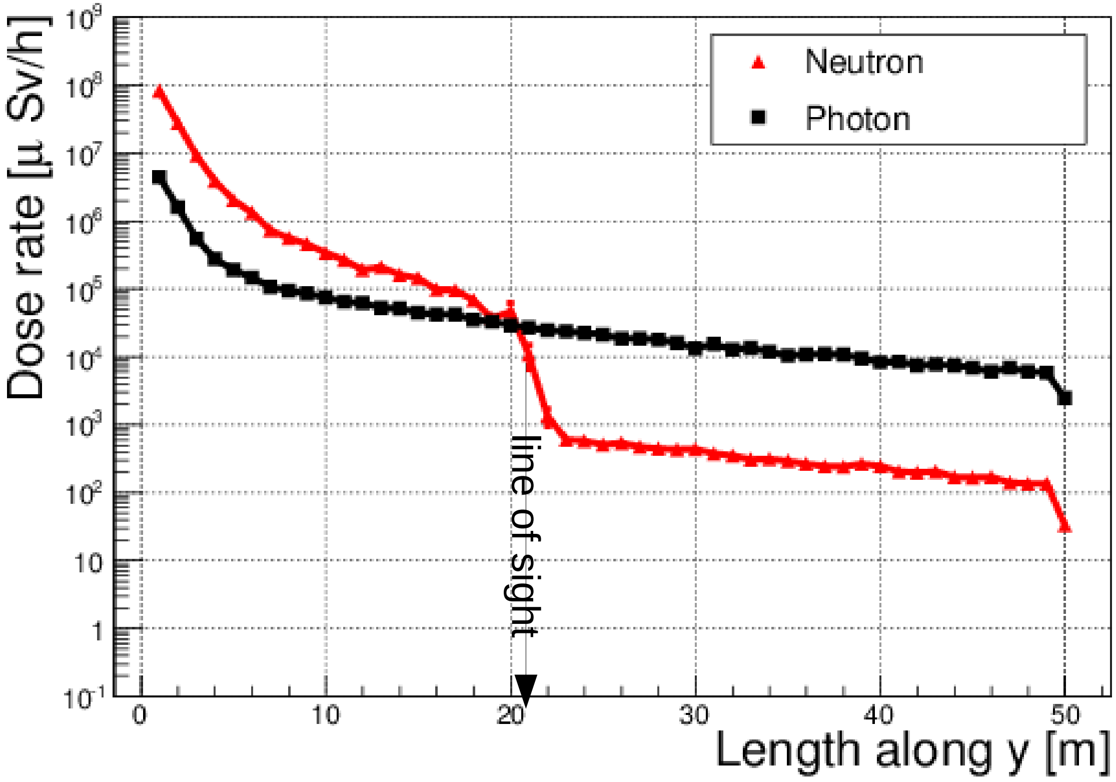


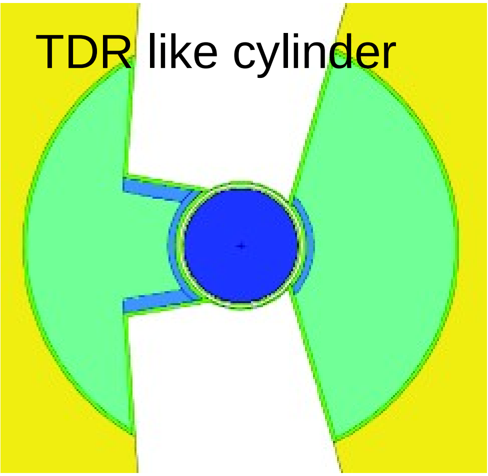
Design status

- ❑ The moderator design at ESS is close to completion

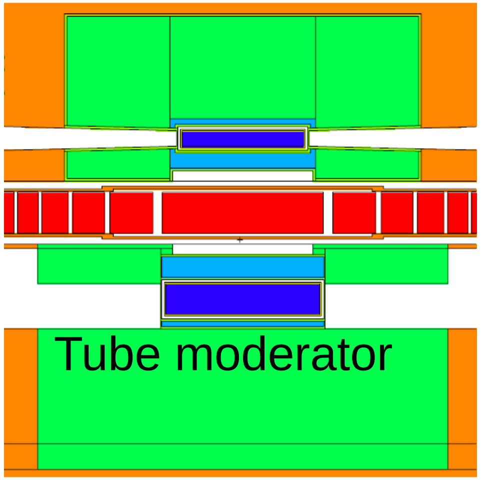
Recommendations from instruments:

- one flat ~3cm moderator above target +
- one taller ~6cm x 6cm below target

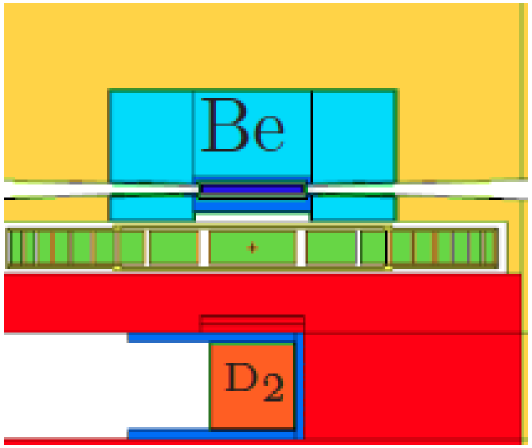
- ❑ Some options for lower moderator are:



Lower moderator, viewed from above



Viewed from the side
More bright than cylinder, but also more directional, and can serve less instr.

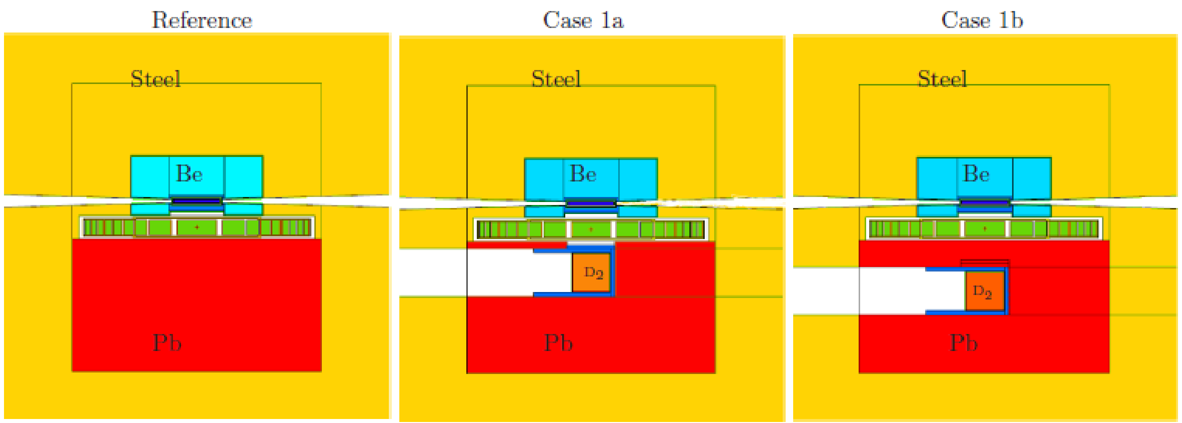


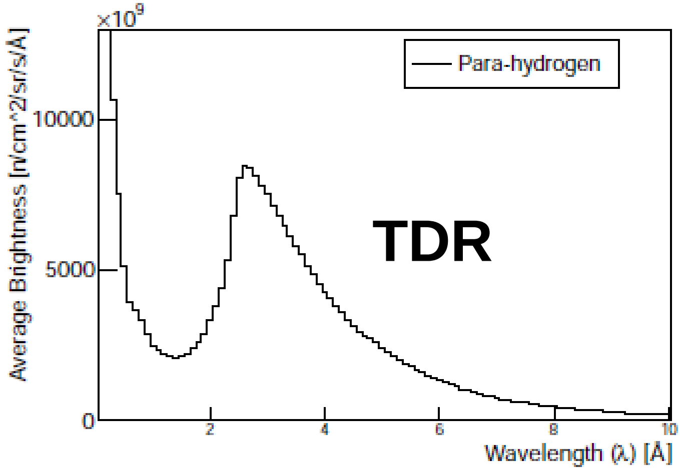
Viewed from the side
Unlikely given the recommendations, but still not excluded. Interesting for nnbar

- ❑ Final decision by October this year

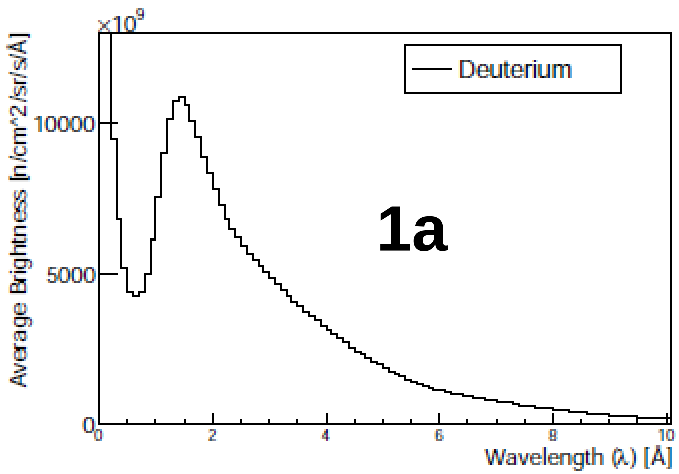
Extra slide :: D2 performance & impact

Example of D_2 moderator – not optimized





Case	Brightness [n/cm^2/sr/s]	
	Volume D_2 moderator (below)	Flat H_2 moderator (above)
Reference		3.34×10^{13}
1a	6.83×10^{12}	2.80×10^{13}
1b	4.56×10^{12}	3.22×10^{13}



Case	$A \times B$ [n/sr/s]
TDR H_2 - 12 cm × 12 cm	1.17×10^{15}
1a D_2 - 25 cm × 20.6 cm	4.27×10^{15}
1b D_2 - 25 cm × 20.6 cm	2.85×10^{15}

- From arXiv:1401.6003

ESS moderator team

- Neutronics Group
  - K. Batkov, E. Klinkby, T. Schönfeldt, A. Takibayev, L. Zanini
- Plus
  - F. Mezei, G. Muhrer, E. Pitcher

Thanks to Phil Bentley for input

Backup slides

Learn more

EUROPEAN SPALLATION SOURCE

Ask me!

Or visit eg:

http://mcstas.org/

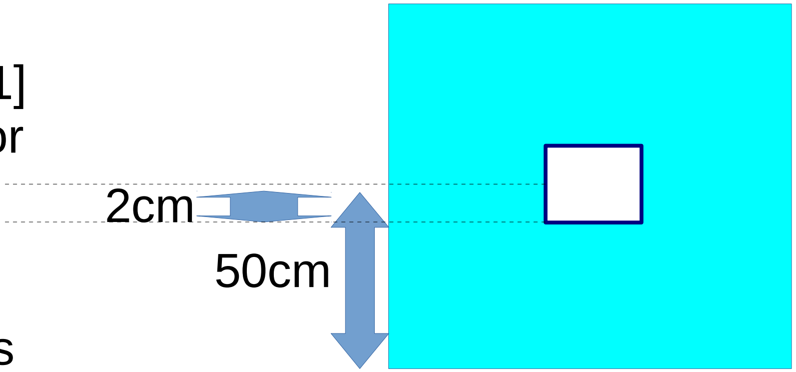
https://svn.mccode.org/svn/GuideBot

[1] E. Klinkby et al. “Interfacing MCNPX and McStas for simulation of neutron transport”. Nucl. Instr & Meth A , 700: p106, 2013.
[2] F. Mezei, et al” Low dimensional neutron moderators for enhanced source brightness”, J. of Neutron Res. 17 (2014) 101–105.
[3] K. Batkov et al, “Unperturbed moderator brightness in pulsed neutron sources”, Nucl Instr. Meth. A 729 (2013) 500.
[4] E. Knudsen et al, “McStas event logger : Definition and applications”. Nucl. Instr & Meth A , 738: p20, 2014.

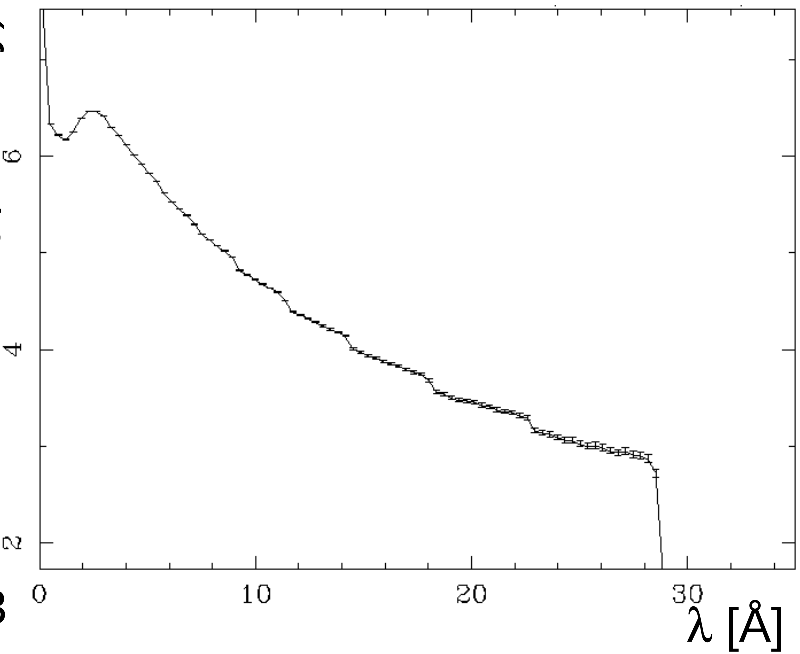
Example: Background along guide

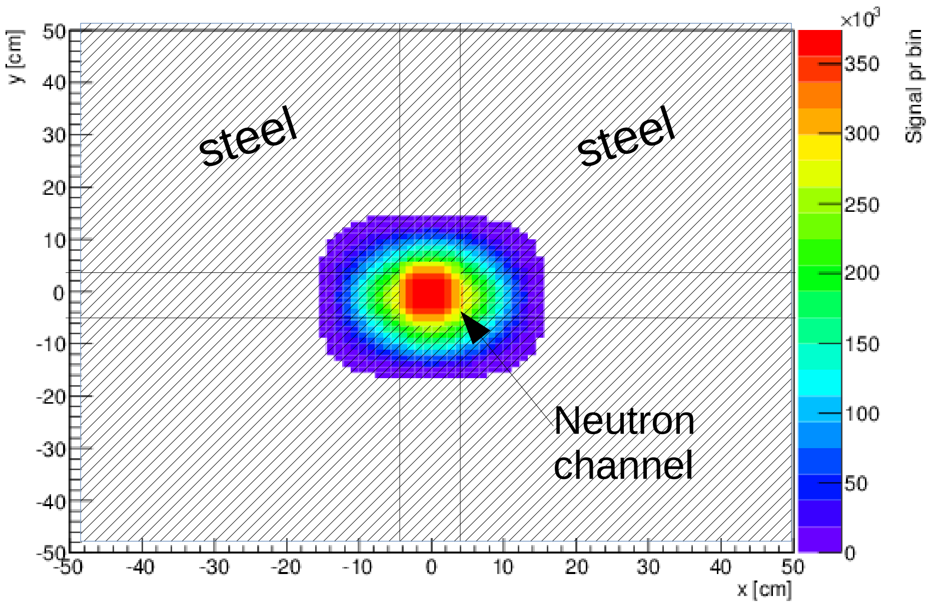
I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface [1]
III. Unreflected neutrons returned to MCNPX for dose-rate calculation

Guide cross-section



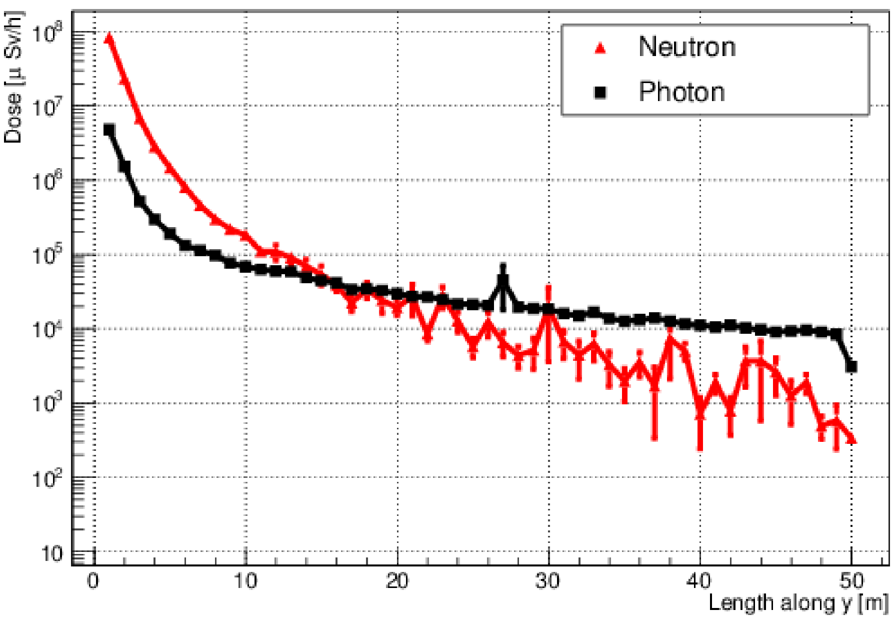
Guide end overilluminated by energetic neutrons



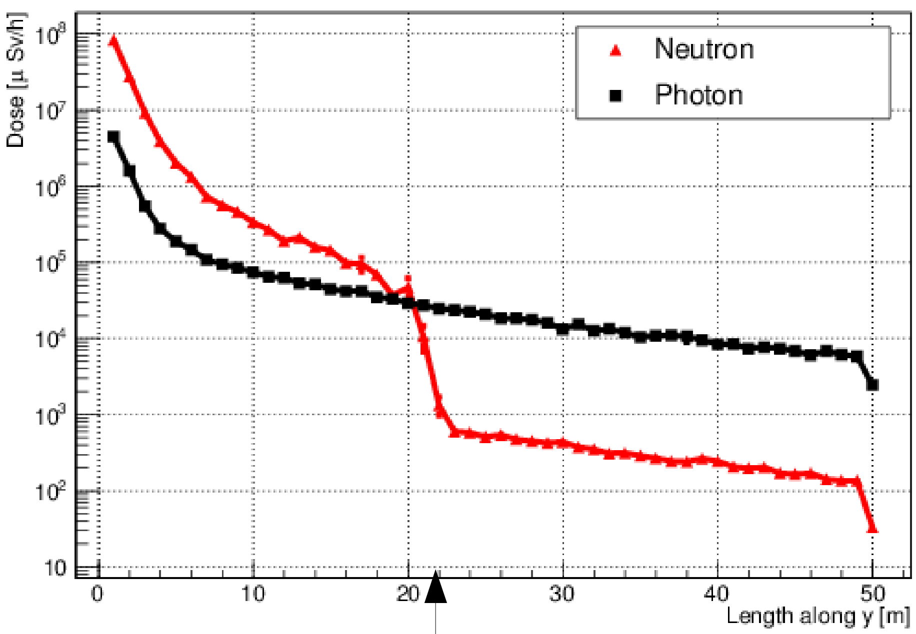


Example: Background along guide

Straight guide



Curved guide ($r_{curvature}$=1500m)

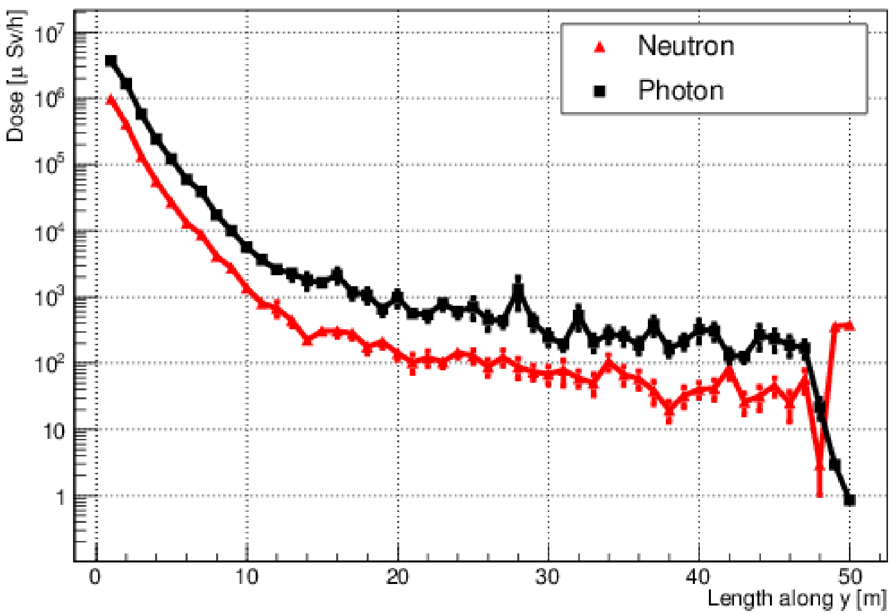


Line-of-sight lost

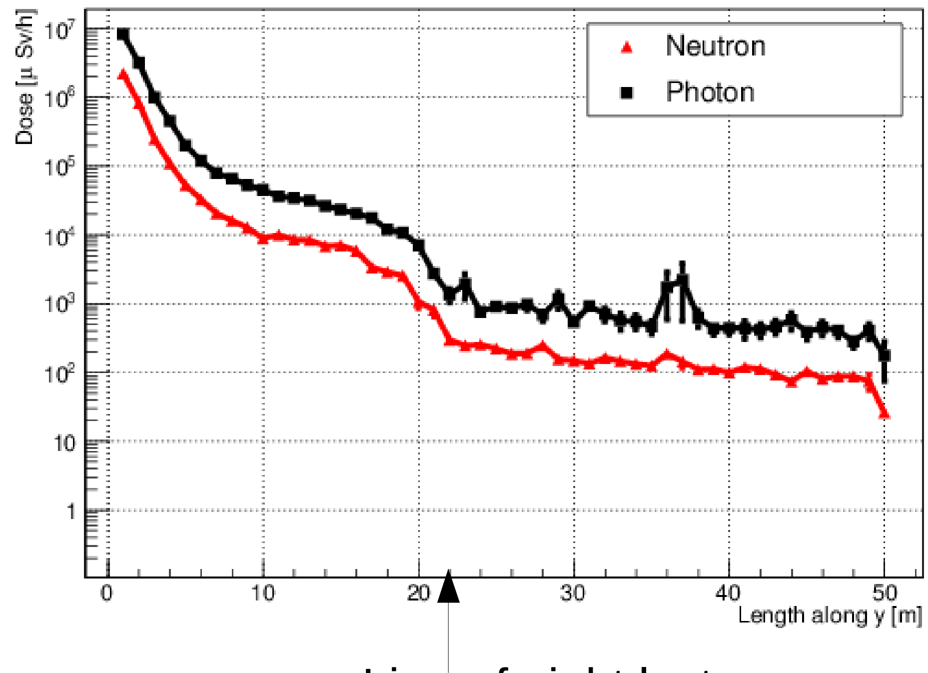
- Dose-rates, measured 5cm in the steel converted from flux according to official Swedish radiation protection procedures

Example: Background along guide

Straight guide



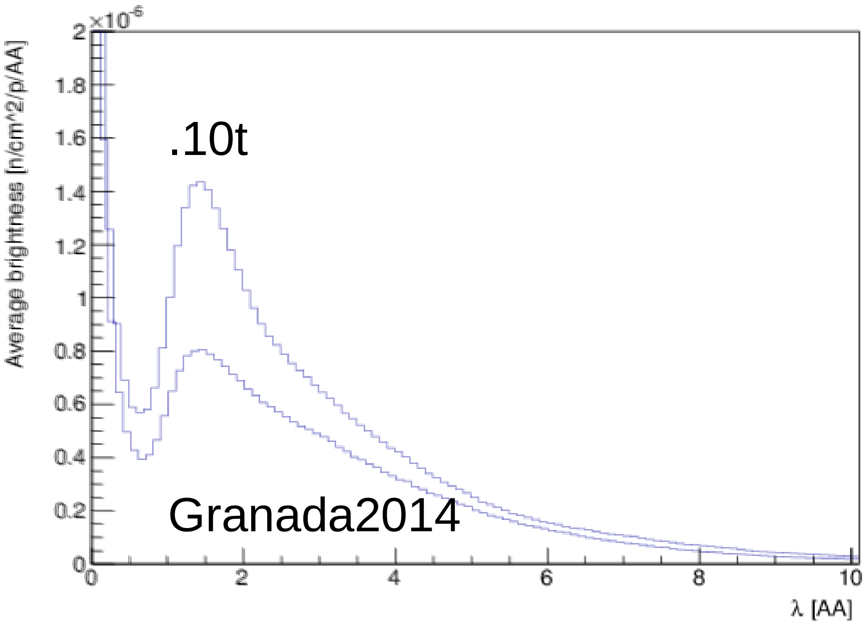
Curved guide ($r_{curvature}$=1500m)

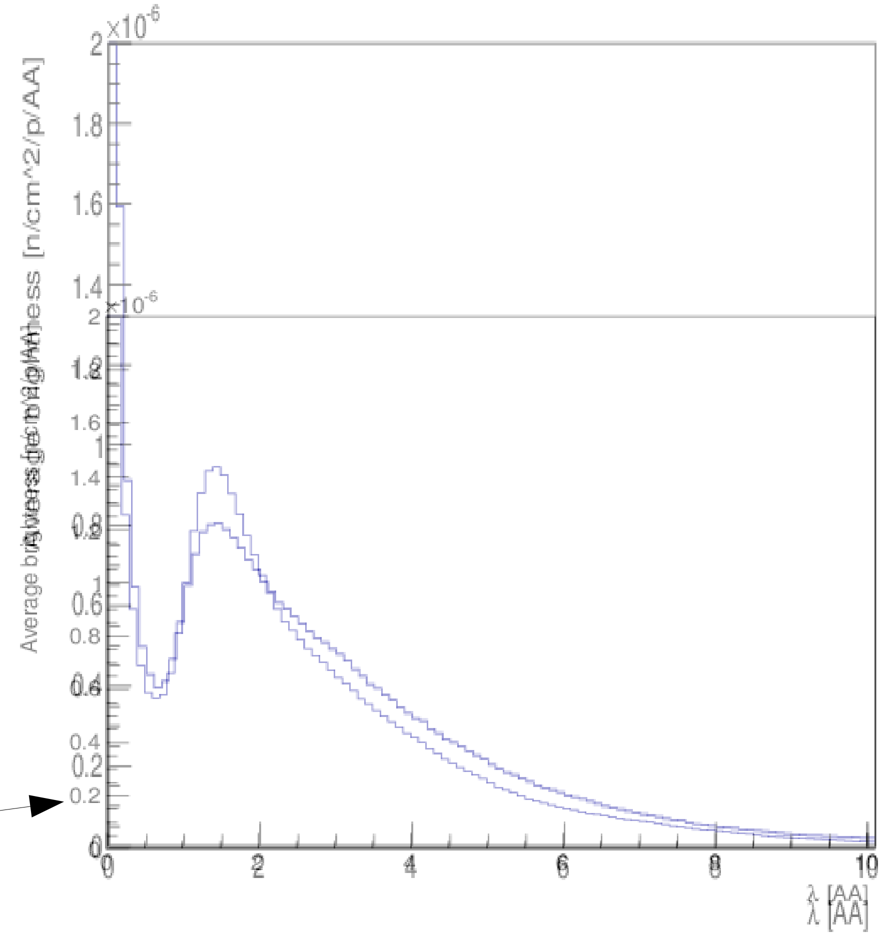


Line-of-sight lost

- Restricting to $\lambda \in \{0.5\ \text{Å} - 1.0\ \text{Å}\}$
- Photon dose-rate follows neutron dose-rate √

Deuterium spectra





Scales are off by about 50%
(comparing 1a to 1b)
→ poor man's rescale