DTU Library

Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

Klinkby, Esben Bryndt; Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Lauritzen, Bent; Nonbøl, Erik; Bentley, Philip; Filges, Uwe

Publication date:
2013

Document Version
Publisher's PDF, also known as Version of record

EUROPEAN SPALLATION SOURCE

Technical University of Denmark

DTU

Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

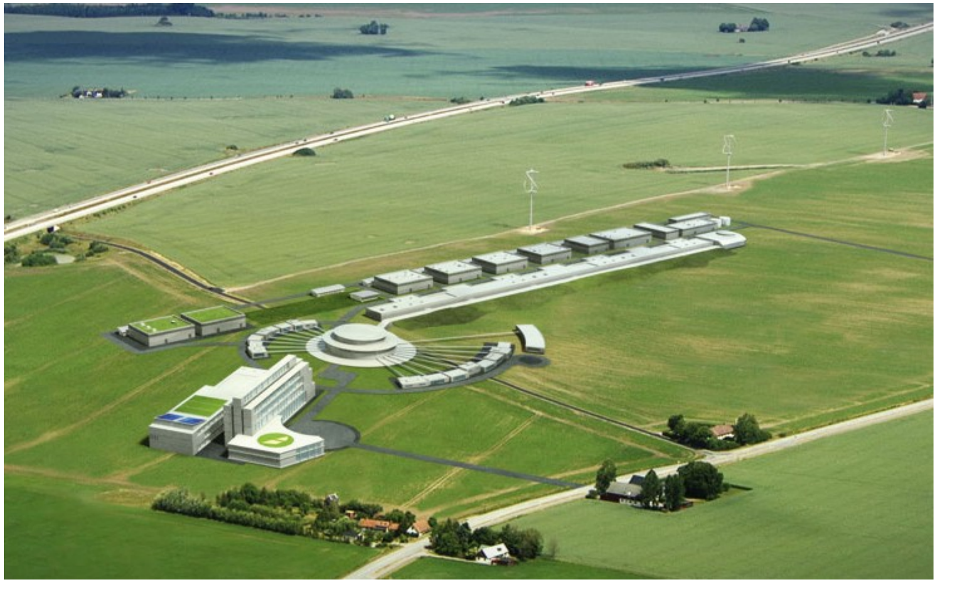
Esben KLINKBY[1,3],

Peter Kjær WILLENDRUP[2,3], Erik Bergbäck KNUDSEN [2,3], Bent LAURITZEN[1,3],
Erik NONBØL[1,3], Phillip BENTLEY[4], Uwe FILGES[5]

1) DTU Nutech, Box 49, 4000 Roskilde, Denmark
2) DTU Physics, Fysikvej 307-312, 2800 Kgs. Lyngby, Denmark
3) ESS design update programme, Denmark
4) European Spallation Source ESS AB, Box 176,S-221 00 Lund, Sweden
5) Paul Scherrer Institut, 5232 Villigen, Switzerland. ESS design update programme, Switzerland

Motivation

- ESS will be a long pulse spallation source and deliver neutrons to 22 instruments located ~20-200m from the target station



⇓

- Guide demands are unprecedented

BUT...

- Guides & shielding is expensive!
- Useful to have a tool that:
  - can monitor where in a guide neutrons are lost
  - allows to optimize reflectivity requirements along a guide
  - serves as an input for dose-rate calculations along guide (n,γ)
  - works within the work-flow accustomed to instrument designers (McStas)
- **McStas Scatterlogger** is the backbone that facilitates this usage

Scatterlogger: Implementation & usage

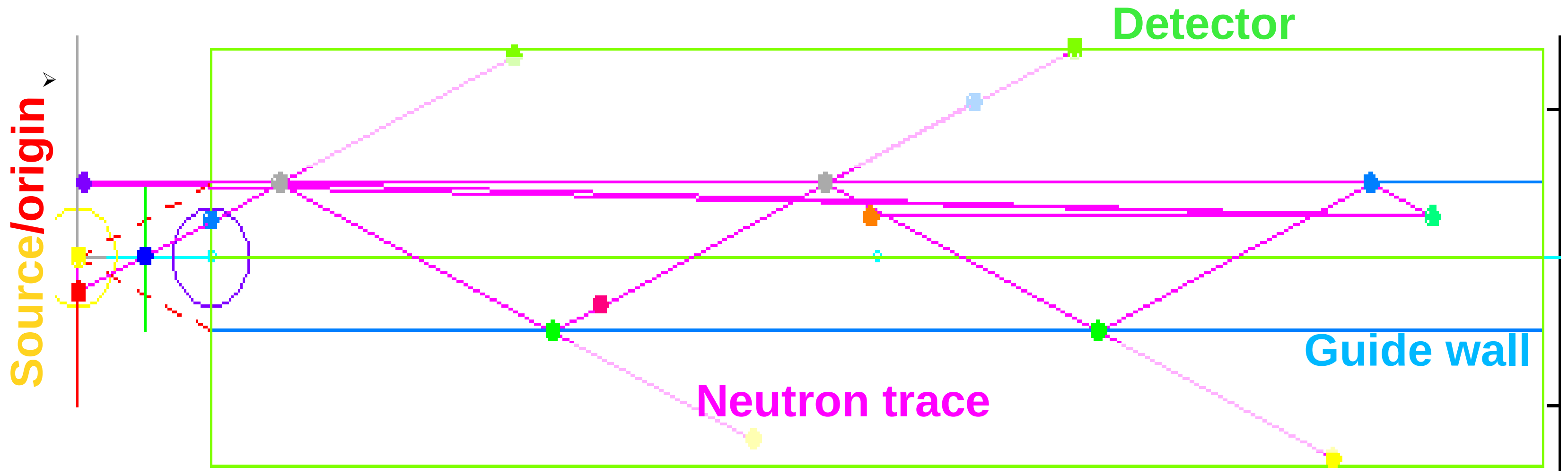
- At each scattering, for any McStas component (eg. a guide), the incoming and outgoing neutron state can be temporally stored & analyzed

At each scattering:

Incomming state: $n_{in} = (\vec{\mathbf{x}}, \vec{\mathbf{v}}_{in}, t, w_{in})$

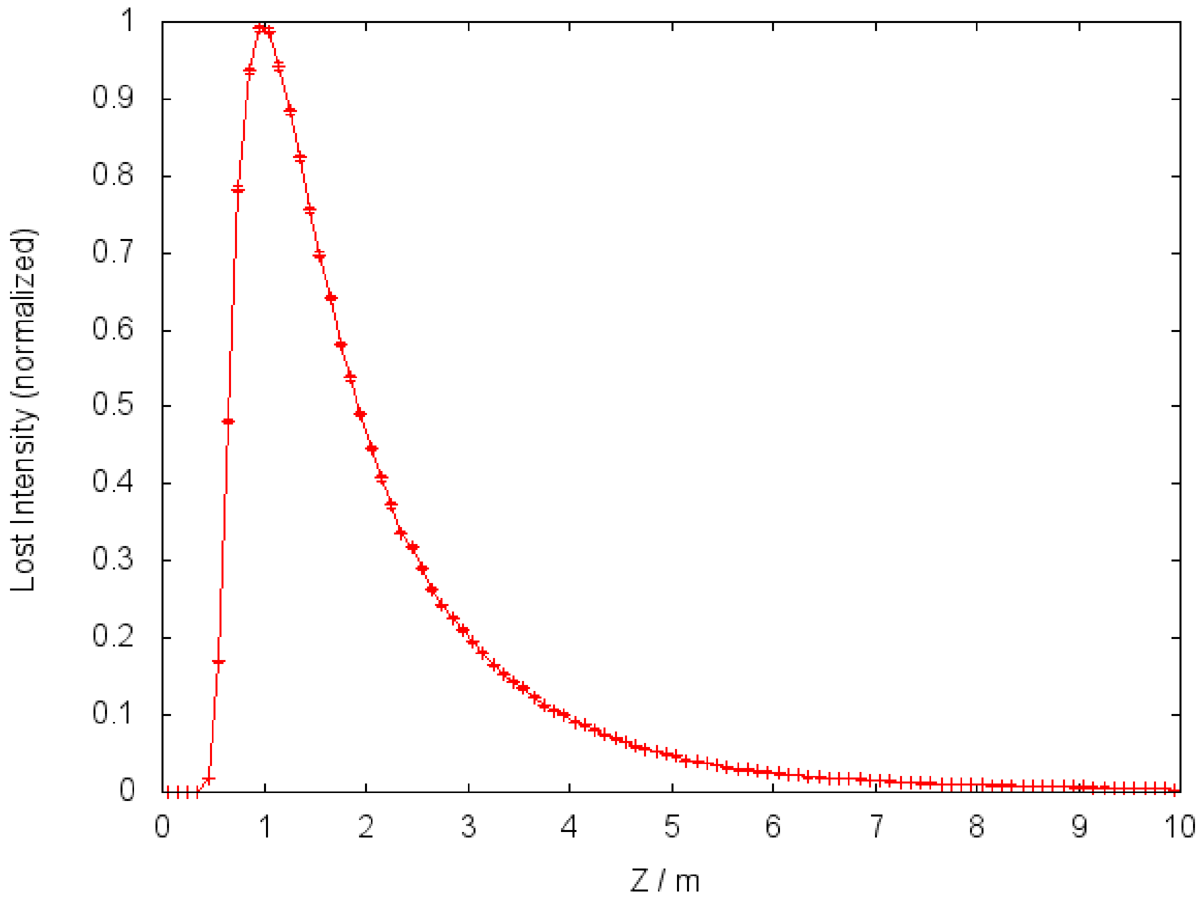
Transmitted state: $n_{trans} = (\vec{\mathbf{x}}, \vec{\mathbf{v}}_{in}, t, w_{trans})$

Reflected state: $n_{refl} = (\vec{\mathbf{x}}, \vec{\mathbf{v}}_{out}, t, w_{in} - w_{itrans})$



Example1: Lost intensity

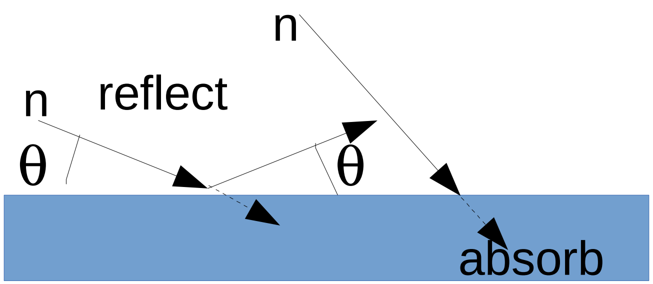
- Lost intensity along guide: w_{trans} *versus* $\vec{x}\cdot\hat{z}$

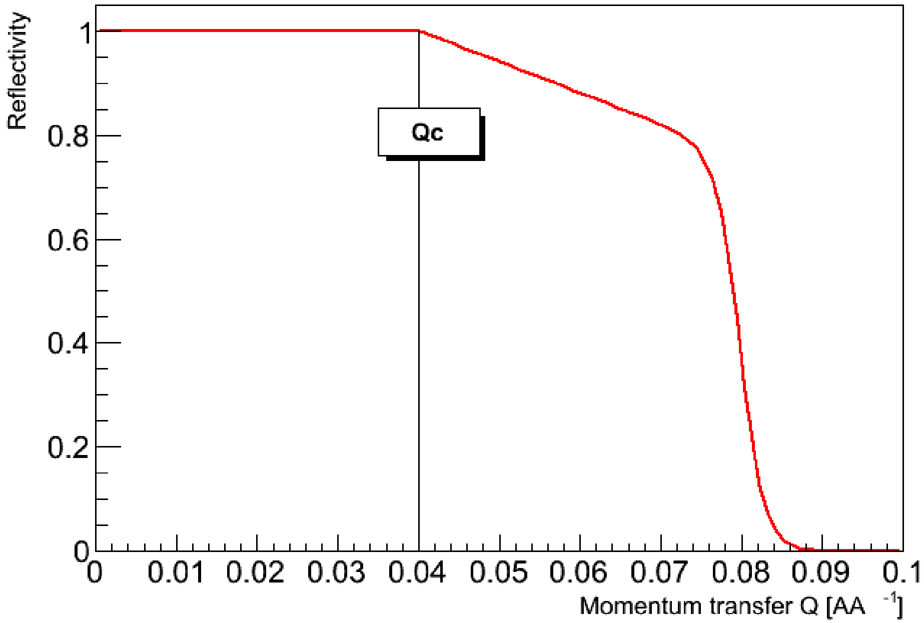


- Depends strongly on specific guide design, and incoming neutrons (i.e. source) spectrum and divergence.

Example2: Reflectivity

- Neutrons are reflected if the energy/incident angle is low enough





$$\cos 2\theta = (\vec{v}_{in} \cdot \vec{v}_{out}) / |\mathbf{v}_{in}|^2$$

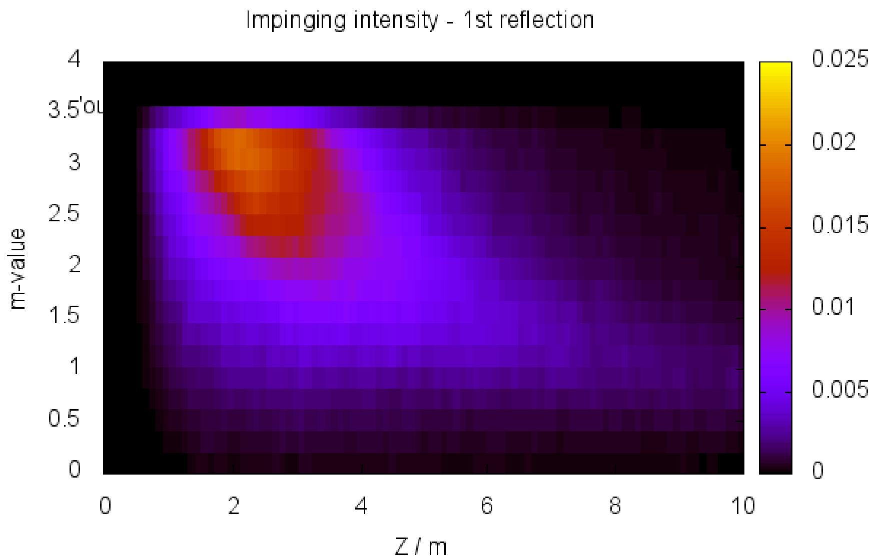
$$k = |\mathbf{v}_{in}| \cdot m_n / \hbar$$

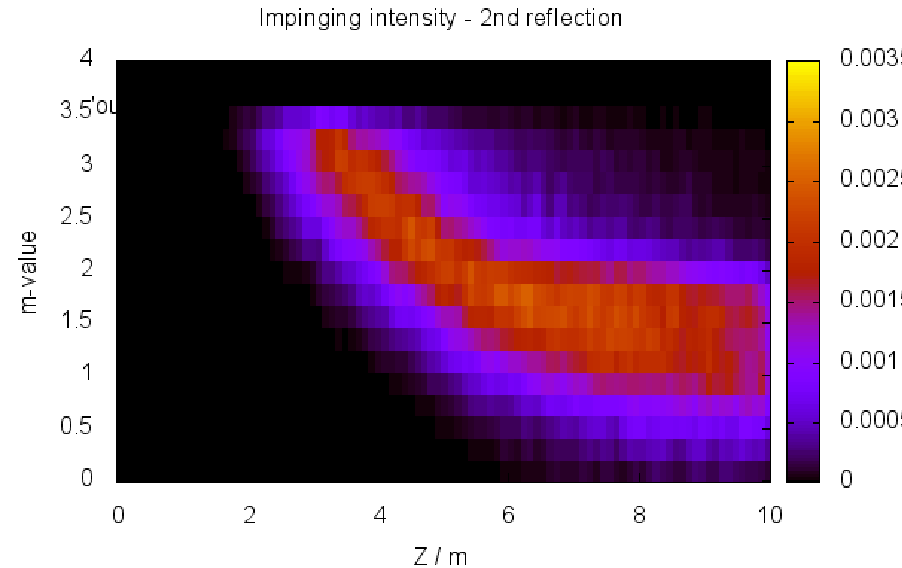
$$\Downarrow$$

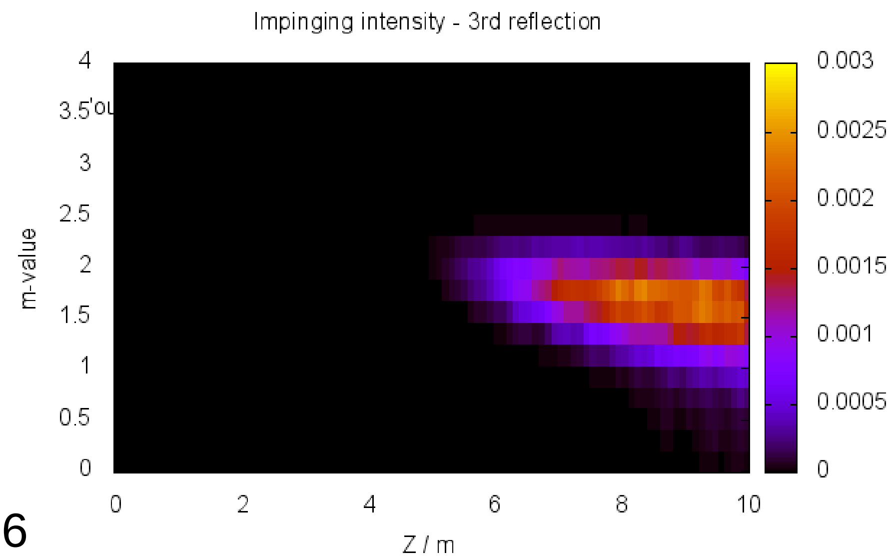
$$m_{min} = 2 \cdot k \cdot \sin(\theta) / 0.0219$$

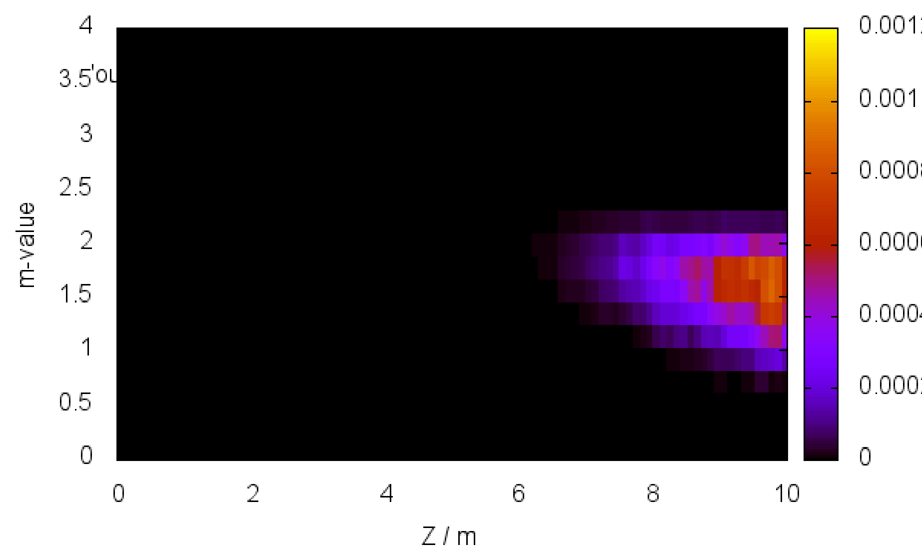
- Given a neutron state and a guide geometry, m_{min} can be calculated at a scattering: The minimum mirror reflectivity requirement which would reflect the neutron without loss

Example2: Reflectivity



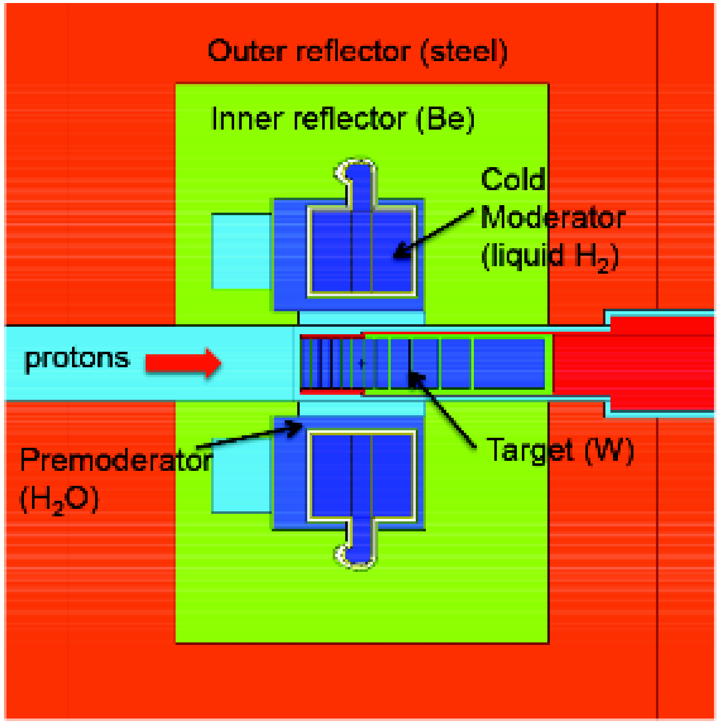


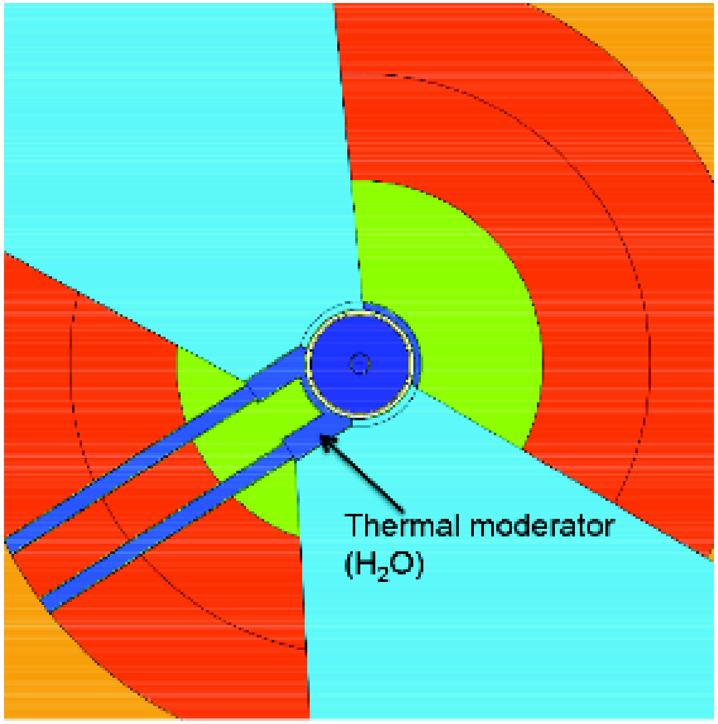




Example3: Background along guide

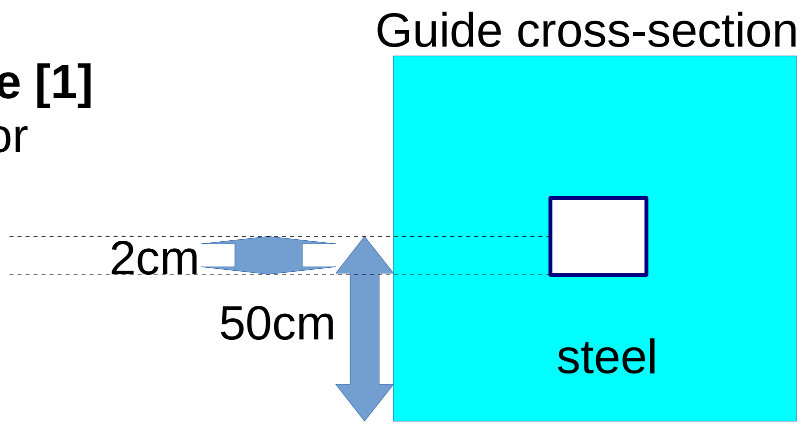
→ **I. Neutrons generated with MCNPX**
II. Handed to McStas through SSW interface [1]
III. Unreflected neutrons returned to MCNPX for dose-rate calculation

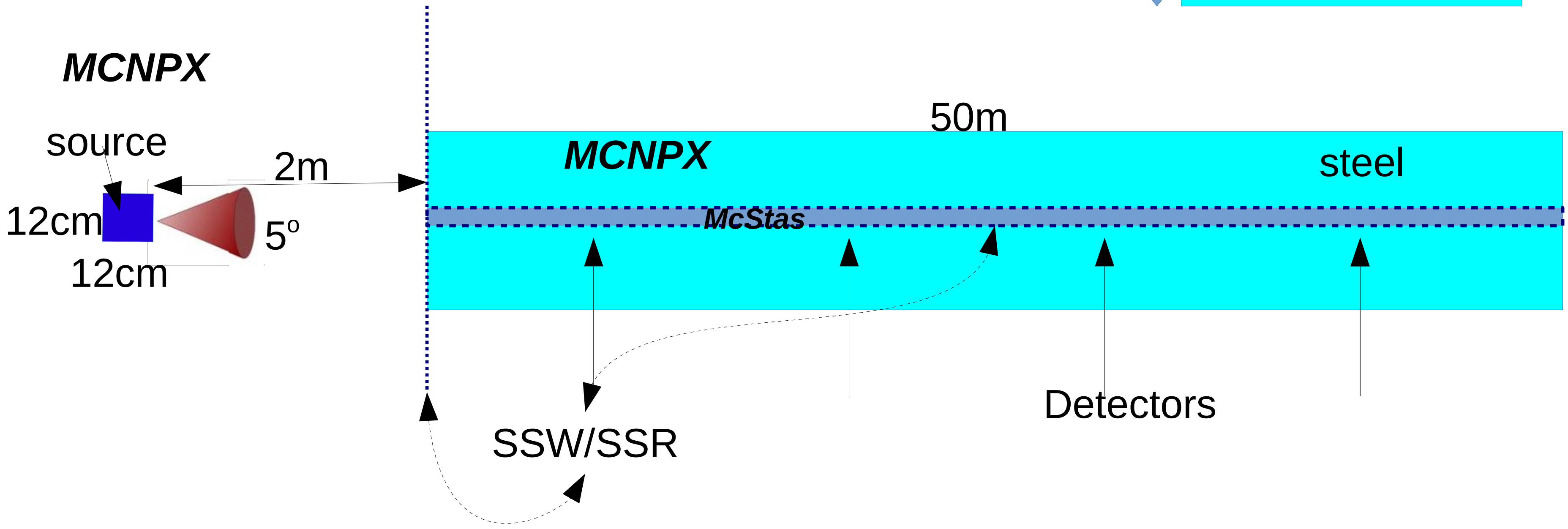




Example3: Background along guide

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

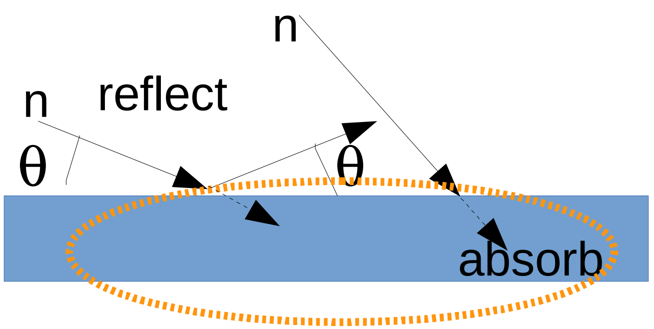




[1] E. Klinkby et al. 'Interfacing MCNPX and McStas for simulation of neutron transport.' Nucl. Instr & Meth A , 700: p106, 2013.

Example3: 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**



<u>At each scattering:</u>

⇒

Incomming state: $n_{in} = (\mathbf{x},\mathbf{v}_{in},t,w_{in})$

Transmitted state: $n_{trans} = (\vec{\mathbf{x}},\vec{\mathbf{v}}_{in},t,w_{trans})$

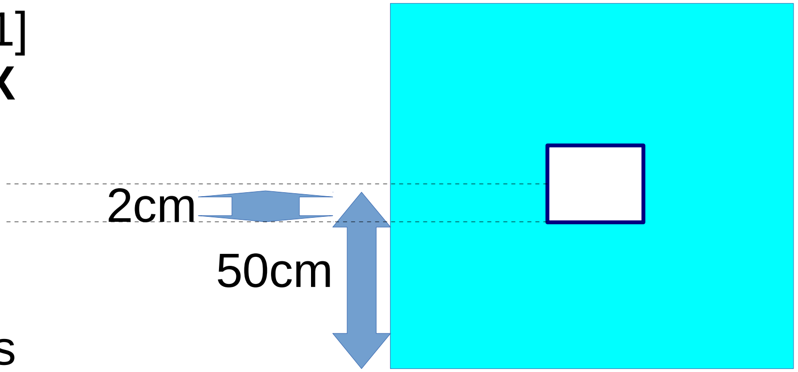
Reflected state: $n_{refl} = (\vec{\mathbf{x}},\vec{\mathbf{v}}_{out},t,w_{in}-w_{itrans})$

➢

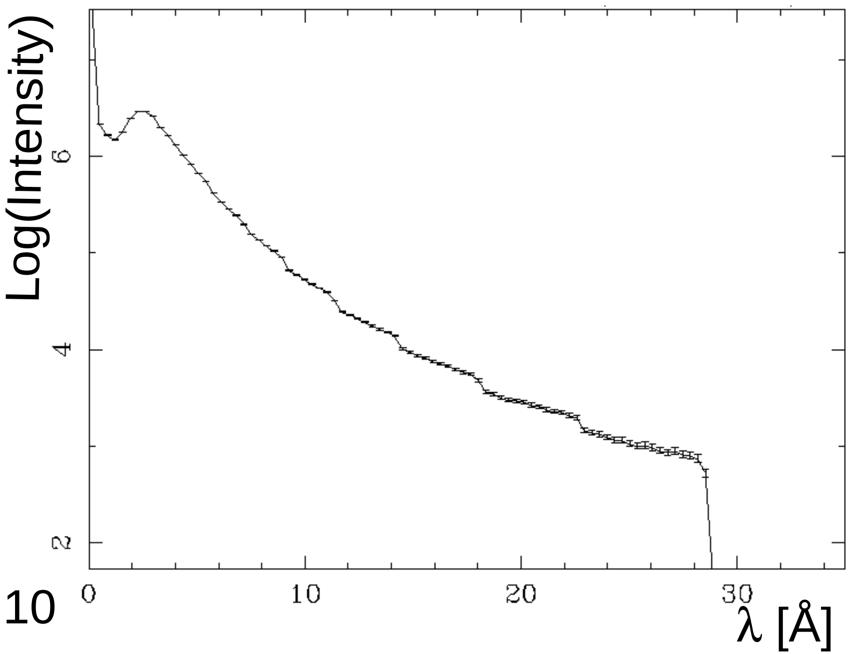
Example3: Background along guide

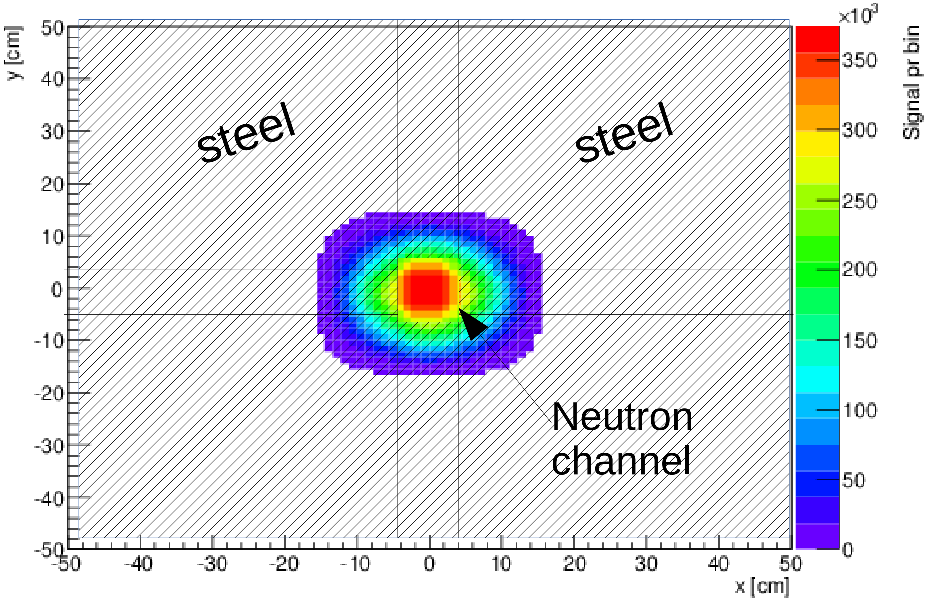
I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface [1]
→ **III. Unreflected neutrons returned to MCNPX for dose-rate calculation**

Guide cross-section



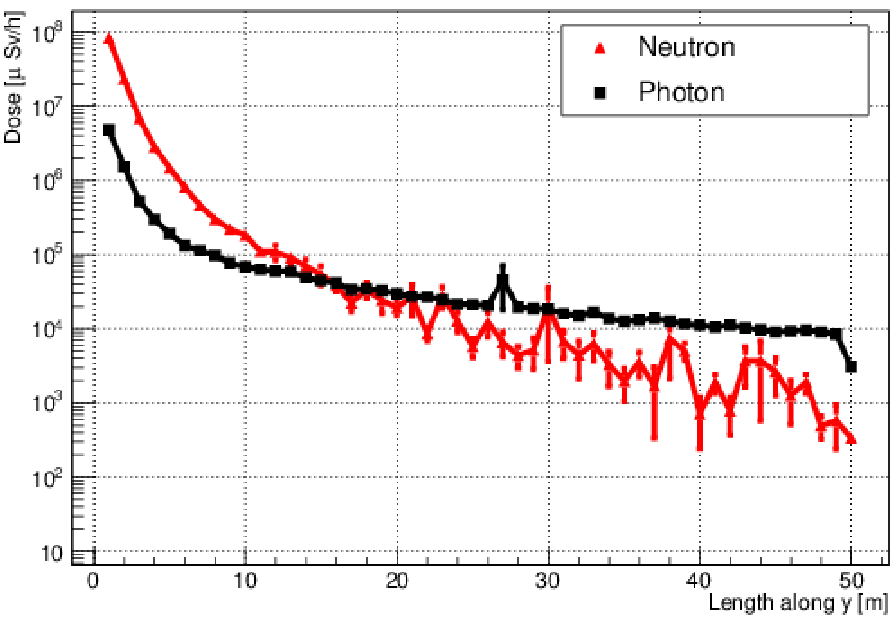
Guide end overilluminated by energetic neutrons



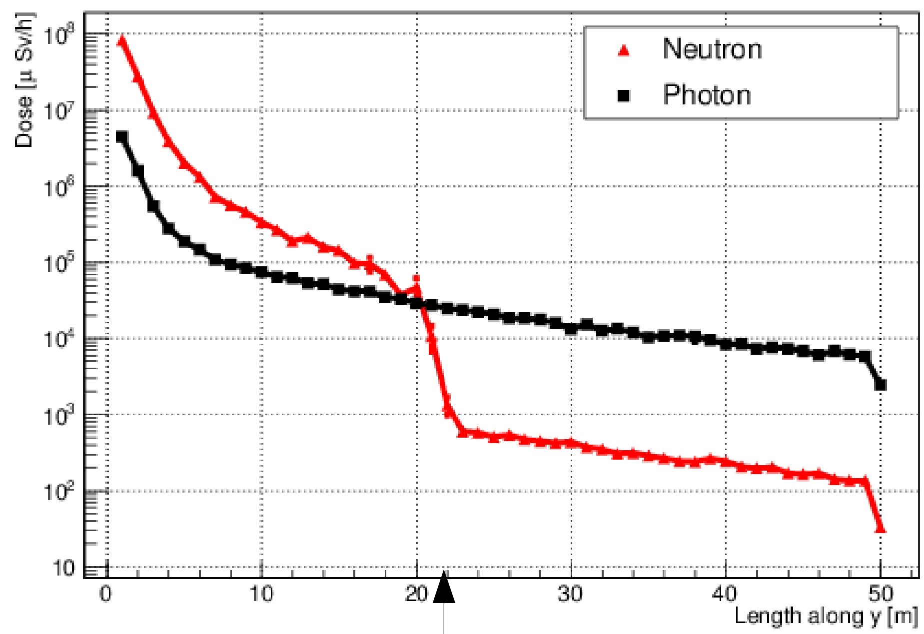


Example3: Background along guide

Straight guide



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

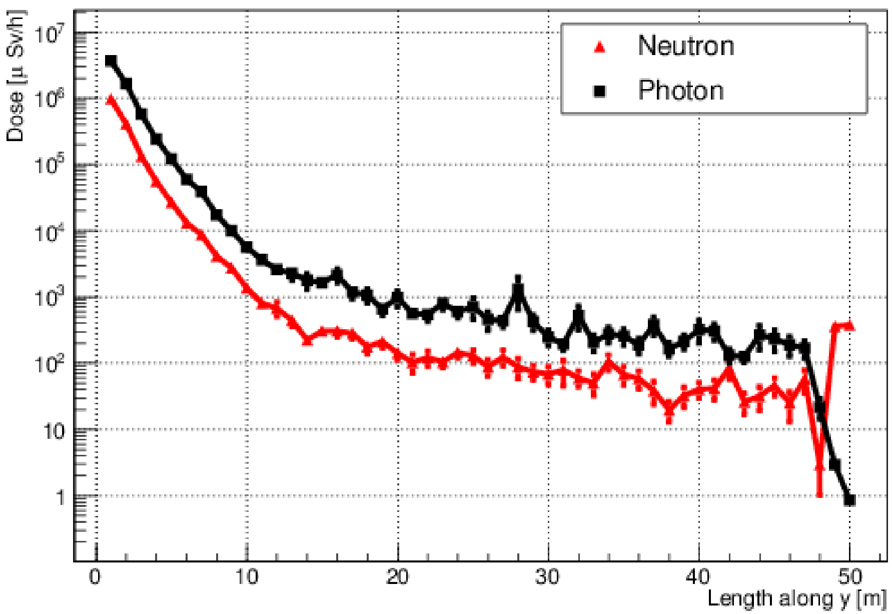


Line-of-sight lost

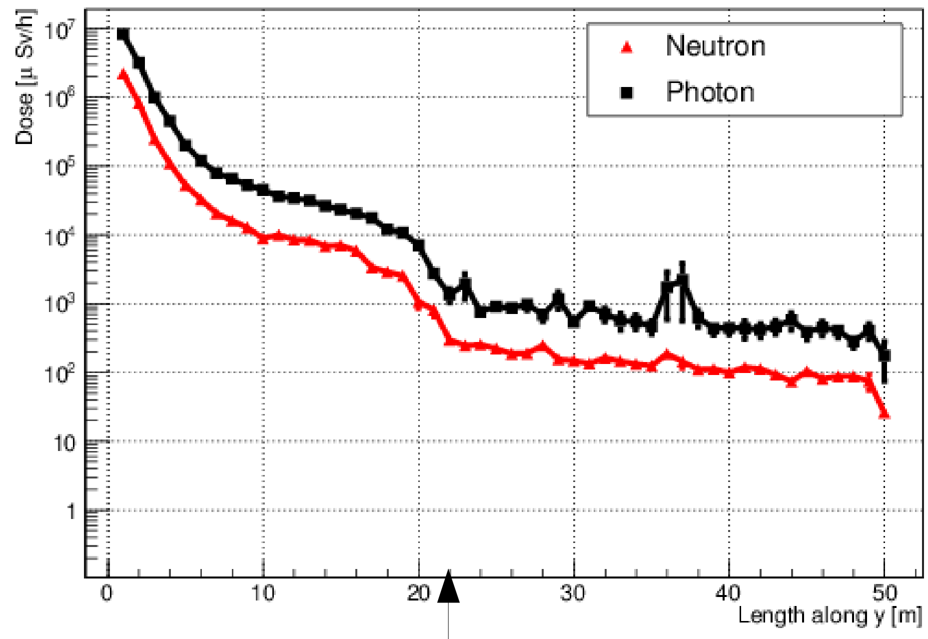
- Dose-rates, measured 5cm in the steel converted from flux according to official Swedish radiation protection procedures

Example3: Background along guide

Straight guide



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

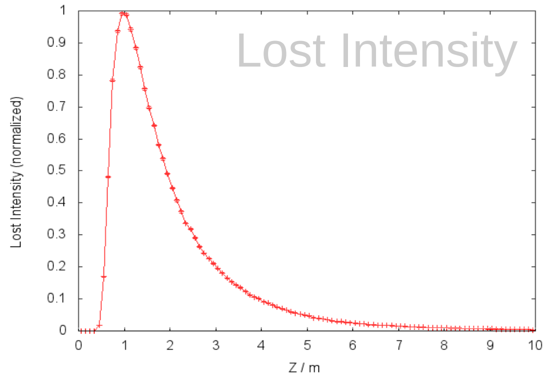


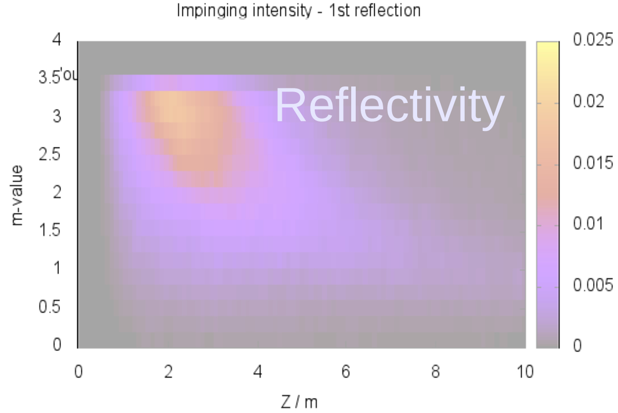
Line-of-sight lost

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

Conclusions

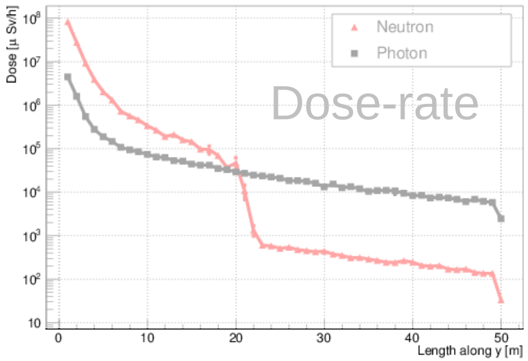
- Logging mechanism useful for guide design:
  - Monitor ***intensity loss***
  - Optimizing use of high/low ***reflectivity*** mirrors
  - Calculate ***dose-rates*** along guide
- Works in instrument designers accustomed work-flow (***McStas***)





Prospects

- Could be used to evaluate gamma and (energetic) neutron background at the sample position / instrument / detectors.
- Must be utilized on an instrument to instrument basis



Backup slides

Reflectivity curve

$$
\begin{aligned}
R &= \frac{R_0}{2}\left(1 - tanh\frac{Q - m \cdot Q_c}{W}\right) \times (1 - \alpha(Q - Q_c)) \qquad for \quad Q > Q_c \\
R &= R_0 \qquad otherwise \qquad (1)
\end{aligned}
$$

where Q is the scattering vector, Q_c is the critical scattering vector, R_0 is the low angle reflectivity constant, W is the width of supermirror cut-off, α is the reflectivity slope, and m is the m-value of the material.

Taken from measurements

Front-end: logger

```
COMPONENT src = Source_simple(
        radius = 0.1, dist = 1, focus_xw = 0.1, focus_yh = 0.1, lambda0=5, dlambda=4.9)
AT (0, 0, 0) RELATIVE Origin

COMPONENT psd0=PSD_monitor(
        xwidth=0.1, yheight=0.1, filename="psd0")
AT(0,0,0.5) RELATIVE PREVIOUS

COMPONENT s1=Scatter_logger()
AT(0,0,1) RELATIVE src

COMPONENT guide_simple = Guide(
        w1 = 0.1, h1 = 0.1, w2 = 0.1, h2 = 0.1, l = 10, R0 = 0.99,
        Qc = 0.0219, alpha = 6.07, m = 2, W = 0.003)
AT (0, 0, 1) RELATIVE src

COMPONENT s2=Scatter_logger_stop(logger=s1)
AT(0,0,0) RELATIVE PREVIOUS
```

Back-end: logger iterator

```
COMPONENT a0=Arm()
AT(0,0,0) ABSOLUTE

COMPONENT iter1 = Scatter_log_iterator()
AT(0,0,0) ABSOLUTE

COMPONENT mnd=Monitor_nD (
        restore_neutron=1, yheight=10, radius=M_SQRT2*0.1,
        options="previous no slit y bins=100", filename="mnd1.dat")
AT(0,0,5) RELATIVE guide_simple
ROTATED (90,0,0) RELATIVE guide_simple

COMPONENT iter2 = Scatter_log_iterator_stop(iterator=iter1)
AT(0,0,0) RELATIVE iter1

COMPONENT a1 = Arm()
AT (0,0,0) ABSOLUTE
JUMP a0 WHEN(MC_GETPAR(iter2,loop))
```

10m setup
- guide & source details

```
COMPONENT Origin = Progress_bar()
AT (0,0,0) ABSOLUTE

COMPONENT src = Source_simple(
   radius = 0.1, dist = 1, focus_xw = 0.1, focus_yh = 0.1, lambda0=5, dlambda=4.9)
AT (0, 0, 0) RELATIVE Origin

COMPONENT psd0=PSD_monitor(
   xwidth=0.1, yheight=0.1, filename="psd0")
AT(0,0,0.5) RELATIVE PREVIOUS

COMPONENT s1=Scatter_logger()
AT(0,0,1) RELATIVE src

COMPONENT guide_simple = Guide(
   w1 = 0.1, h1 = 0.1, w2 = 0.1, h2 = 0.1, l = 10, R0 = 0.99,
   Qc = 0.0219, alpha = 6.07, m = 2, W = 0.003)
AT (0, 0, 1) RELATIVE src
```

m-value calculation

```
double mvalue;
int reflc;
int reflect_m-value(double *ns_tilde, struct Generalized_State_t *S0, struct Generalized_State_t *S1){
      /*position comes from "new" state*/
      ns_tilde[0]=S1->_x;ns_tilde[1]=S1->_y;ns_tilde[2]=S1->_z;
      /*velocity is the "old" state*/
      ns_tilde[3]=S0->_vx;ns_tilde[4]=S0->_vy;ns_tilde[5]=S0->_vz;
      /*time from new*/
      ns_tilde[6]=S1->_t;
      /*weight is impinging weight - old state*/
      ns_tilde[10]=S0->_p;

      double v = sqrt(S0->_vx*S0->_vx+S0->_vy*S0->_vy+S0->_vz*S0->_vz);
      double k = v*V2K;
      double theta  = 0.5*acos(scalar_prod(S0->_vx,S0->_vy,S0->_vz,S1->_vx,S1->_vy,S1->_vz)/(v*v));
      mvalue = 2*k*sin(theta)/0.0219;
      reflc=S1->_idx;
      return 0;
}
```

Another example: Specialized pseudo neutron state function → background along guide

Same as before

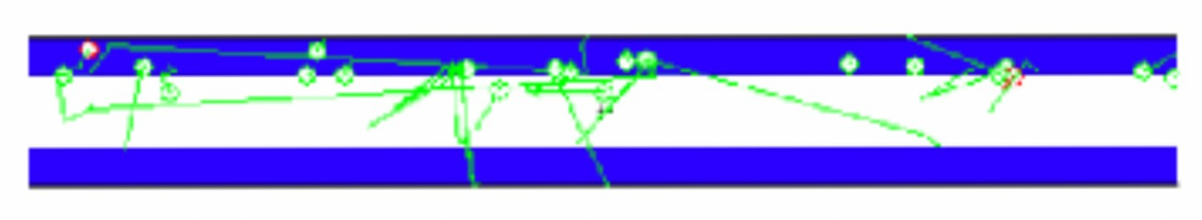
```
/*position comes from "new" state*/
ns_tilde[0]=S1->_x;ns_tilde[1]=S1->_y;ns_tilde[2]=S1->_z;

/*velocity is the "old" state*/
ns_tilde[3]=S0->_vx;ns_tilde[4]=S0->_vy;ns_tilde[5]=S0->_vz;

/*time from new*/
ns_tilde[6]=S1->_t;
/*weight is difference old-new to mean the neutrons "deposited" in the guide wall*/
ns_tilde[10]=S0->_p-S1->_p;
```

I.e.: The temporarily stored state is the ***un-reflected neutrons*** - normally discarded

Using the MCNPX-McStas interface: *Virtual_MCNP_ss_output.comp* (McStas 2.0), the simulation of absorbed neutrons proceeds:



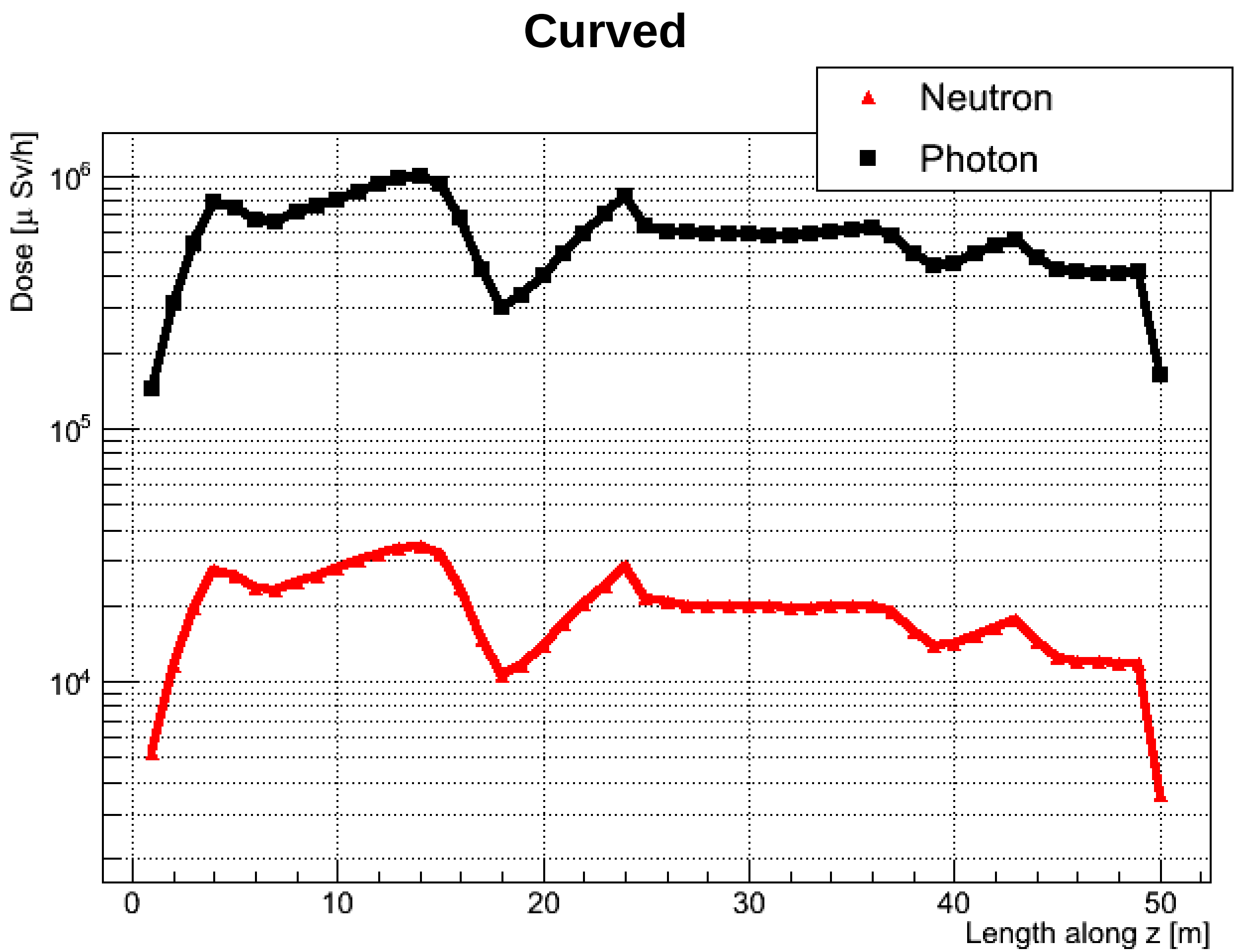
Neutron and gamma trajectories (a few example events from MCNPX → Vised)

Next: use to calculate shielding requirements for realistic ESS guide geometry and source

New source – cold pencil

- ***Guide starts at z=200cm***
- c Source definition: cold, in guide opening
- sdef x=d2 y=d3 z=0.0 dir=d4 vec=0 0 1 erg=1e-8 par=n
- si2 h -1.0 1.0
- sp2 0 1
- si3 h -1.0 1.0
- sp3 0 1
- si4 h 0.99999 1 $~0.25grad
- sp4 0 1

Dose rates: cold-pencil-beam

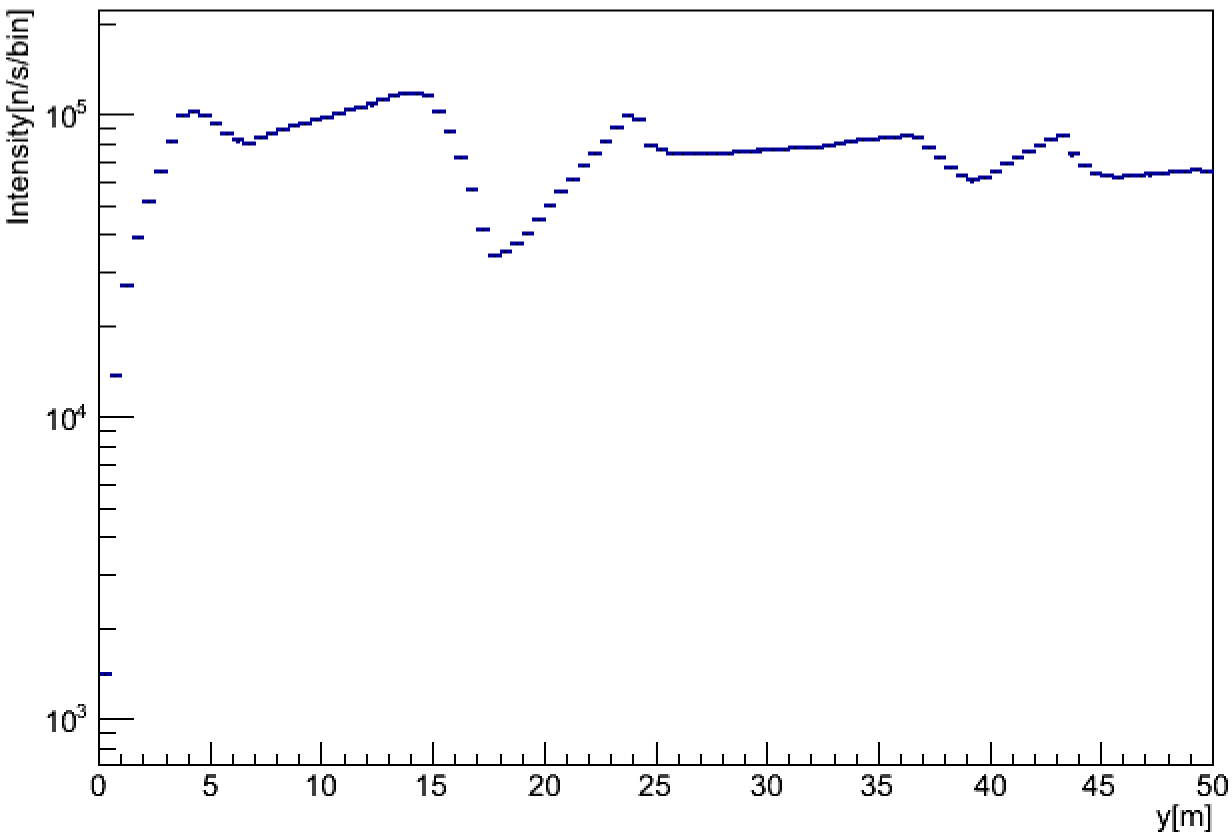


i.e. perfect match between curve structure

Q: how thus this match McStas-only treatment showing intensity loss?

McStas-only treatment: intensity loss

(pencil-cold-beam)



Better validation example

- Using same geometry, but limit MCNPX source to [0.5-1]Å
- λ range chosen such that
  - ~half the neutrons should be absorbed.
  - Avoid high energy, high intensity peak (showers!), not drawn by exp and $1/r^2$ fall of, of energetic gammas.