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

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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

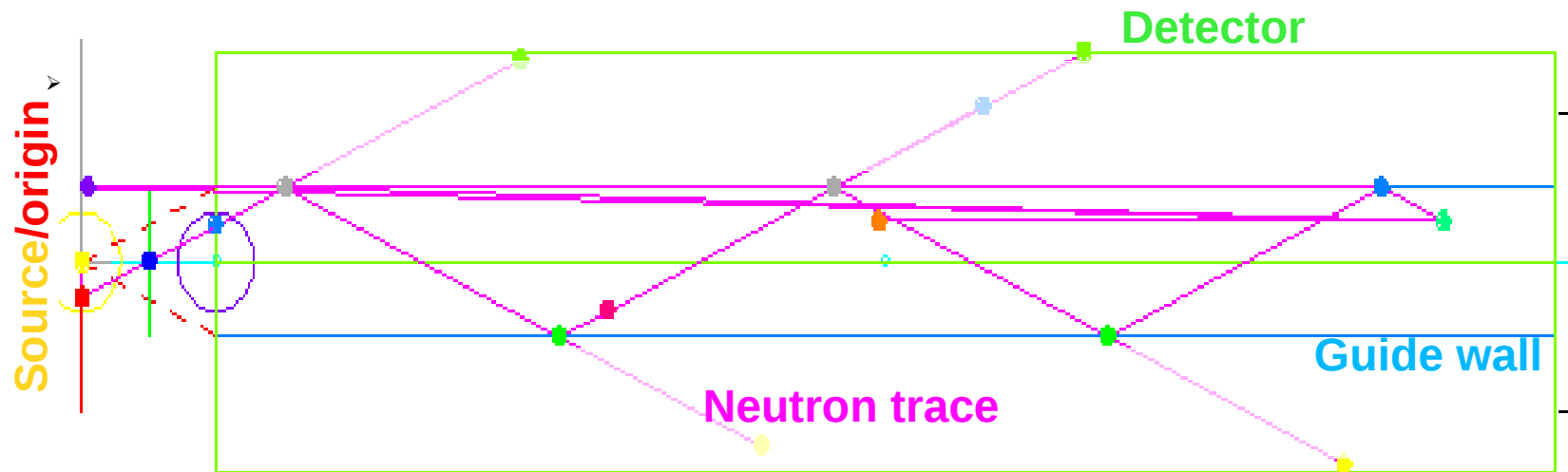
- At each scattering, for any McStas component (eg. a guide), the incoming and outgoing neutron state can be temporally stored & analyzed

At each scattering:

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

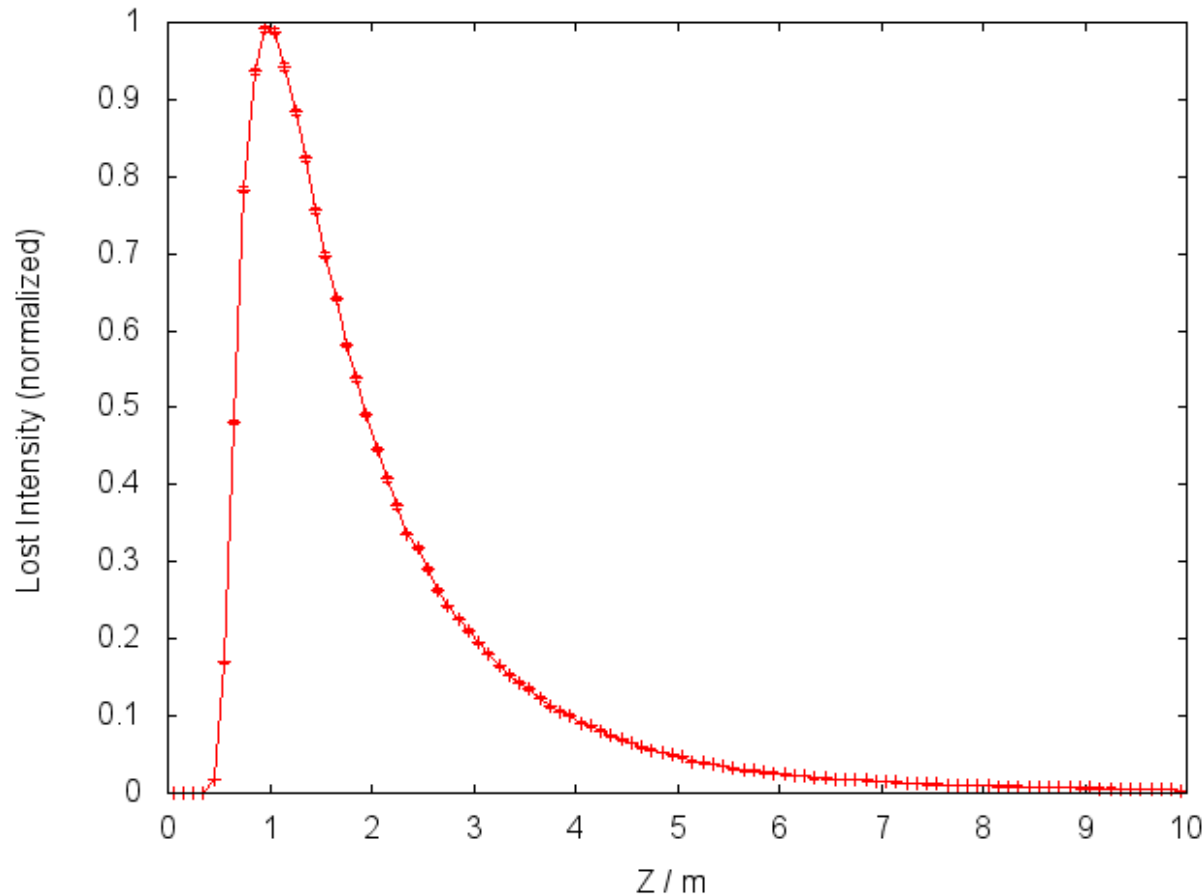
Transmitted state: $n_{trans} = (\vec{x}, \vec{v}_{in}, t, w_{trans})$

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



Example1: Lost intensity

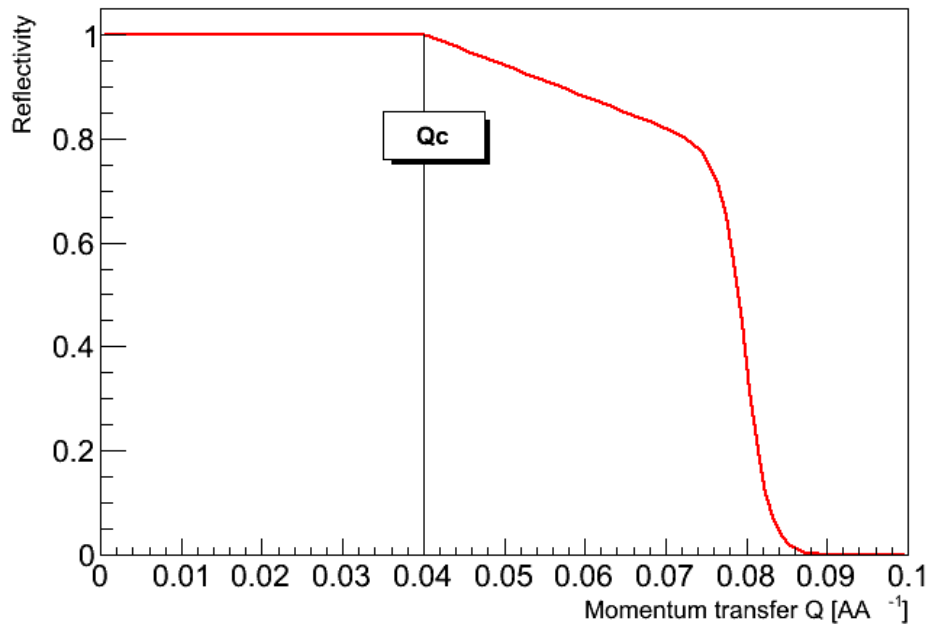
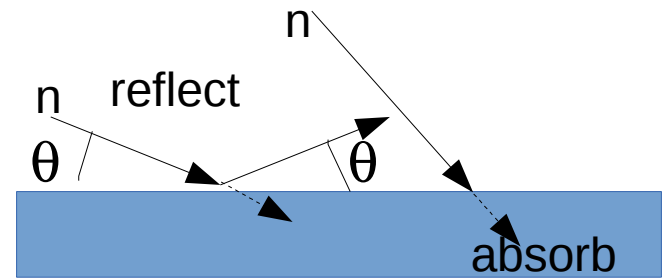
- Lost intensity along guide: w_{trans} versus $\vec{x} \cdot \hat{z}$



- 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



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

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

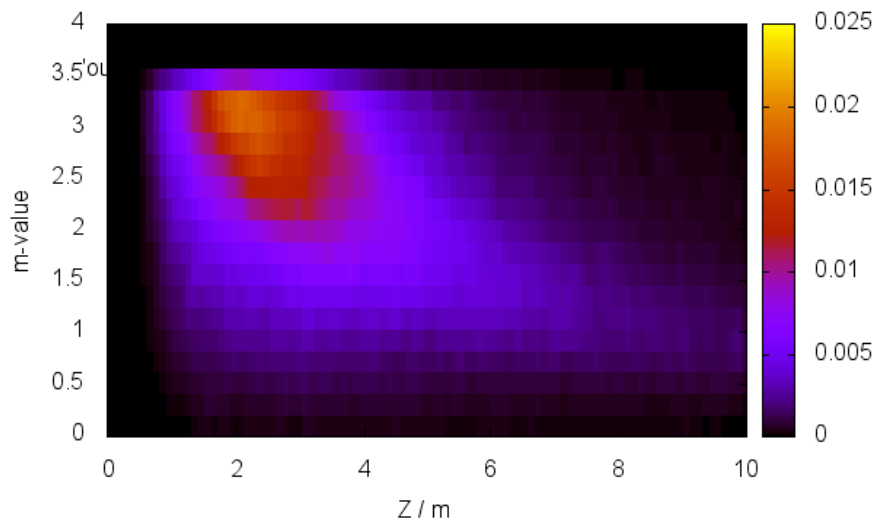
$$\Downarrow$$

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

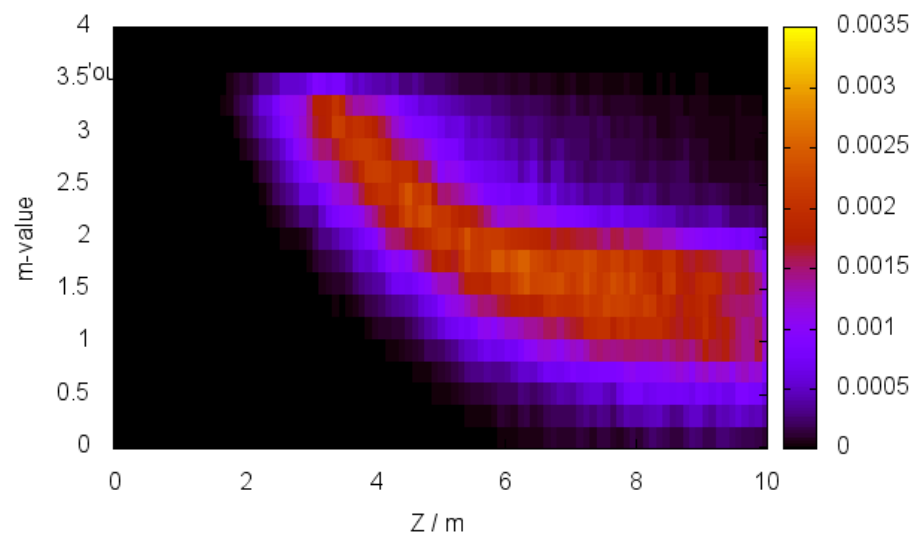
- Given a neutron state and a guide geometry, m_{min} can be calculated at a scattering: The minimum mirror reflectivity requirement which would reflect the neutron without loss

Example2: Reflectivity

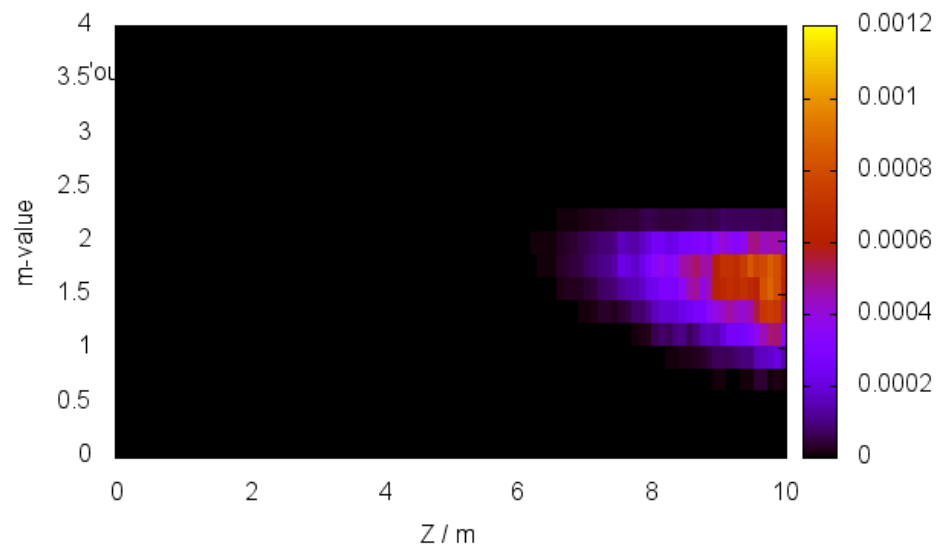
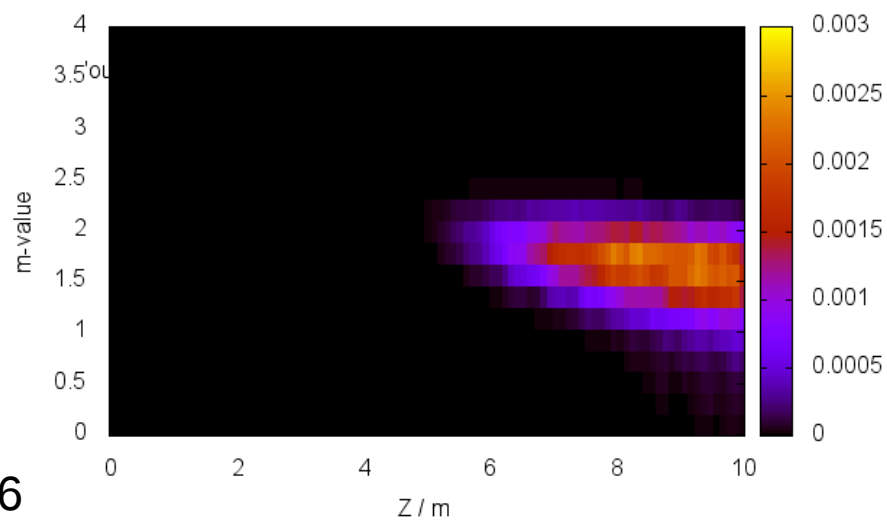
Impinging intensity - 1st reflection



Impinging intensity - 2nd reflection

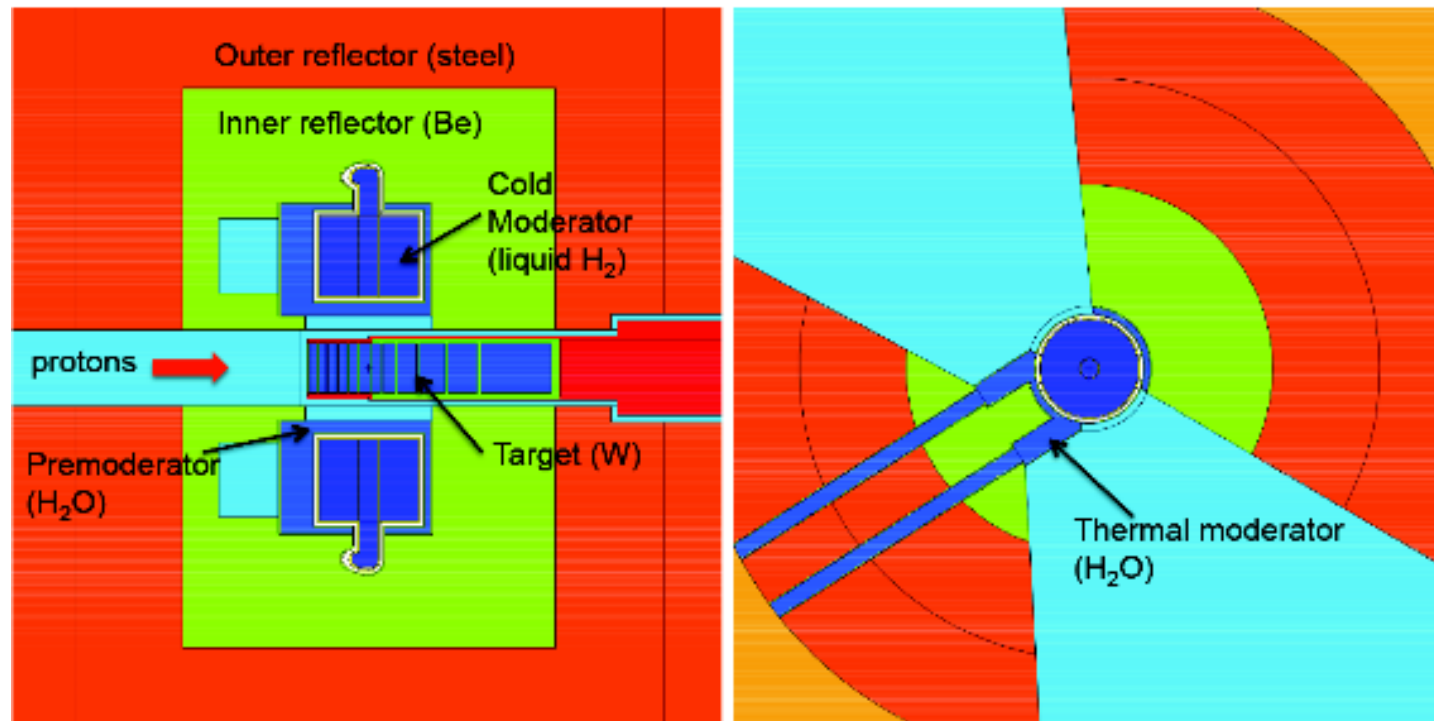


Impinging intensity - 3rd reflection



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

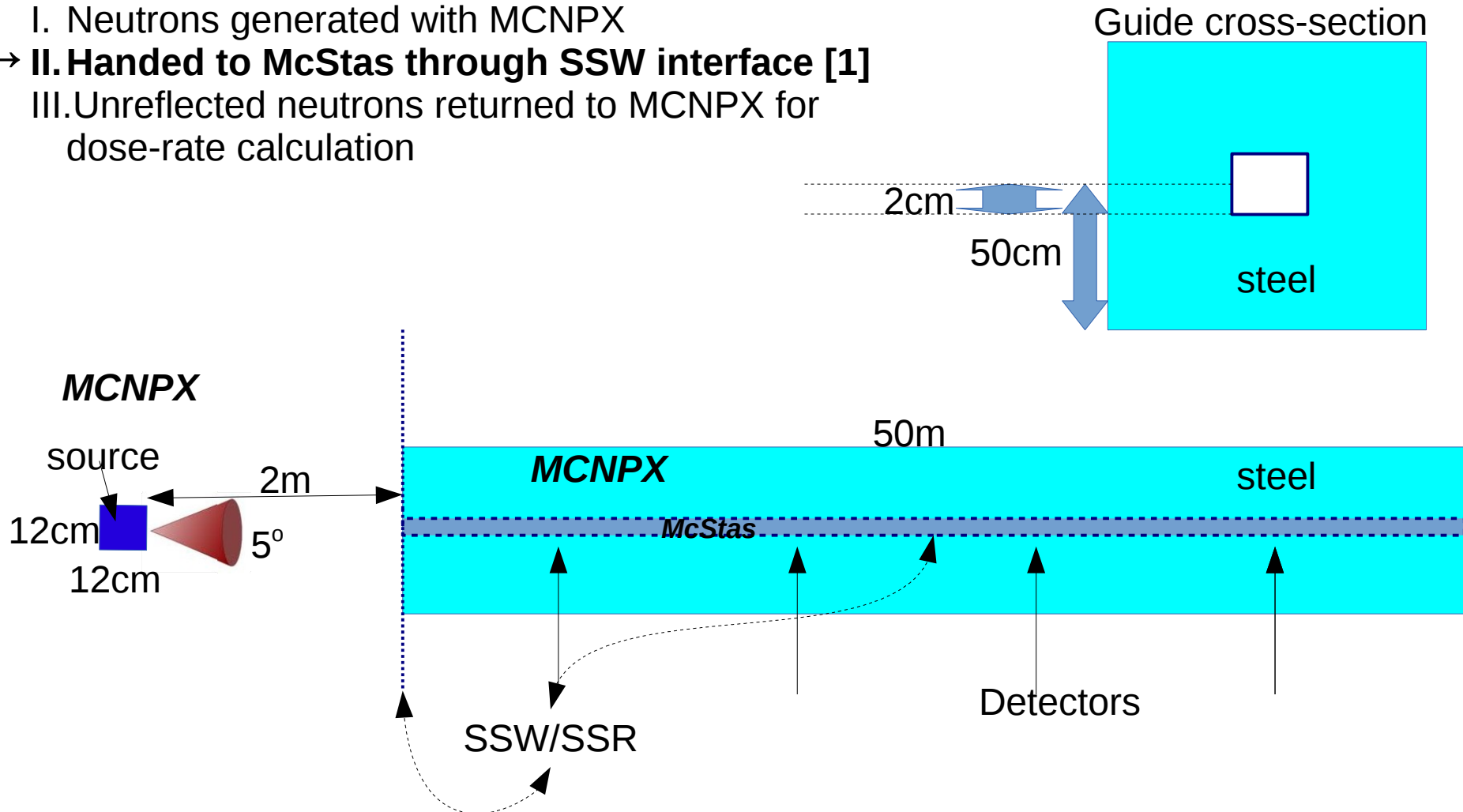


Example3: Background along guide

I. Neutrons generated with MCNPX

→ II. Handed to McStas through SSW interface [1]

III. Unreflected neutrons returned to MCNPX for dose-rate calculation



Example3: Background along guide

I. Neutrons generated with MCNPX

II. Handed to McStas through SSW interface [1]

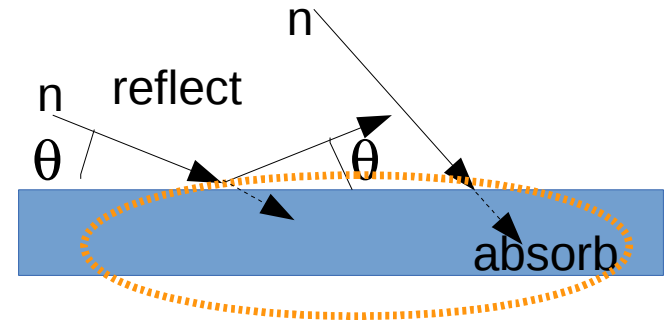
→ III. **Unreflected neutrons returned to MCNPX for dose-rate calculation**

At each scattering:

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

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

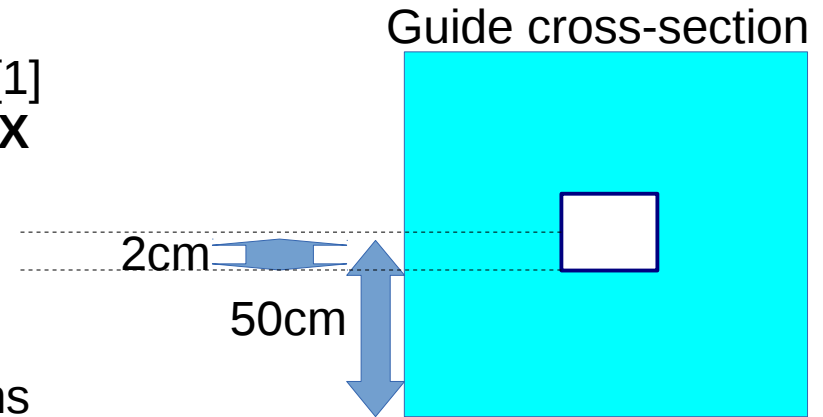
Reflected state: $n_{refl} = (\vec{\mathbf{x}}, \vec{\mathbf{v}}_{out}, t, w_{in} - w_{itrans})$



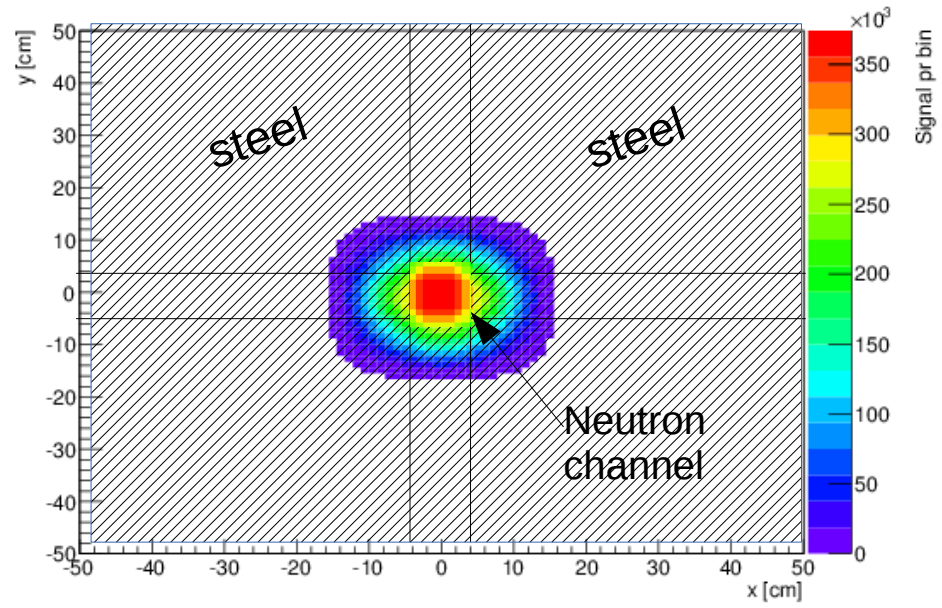
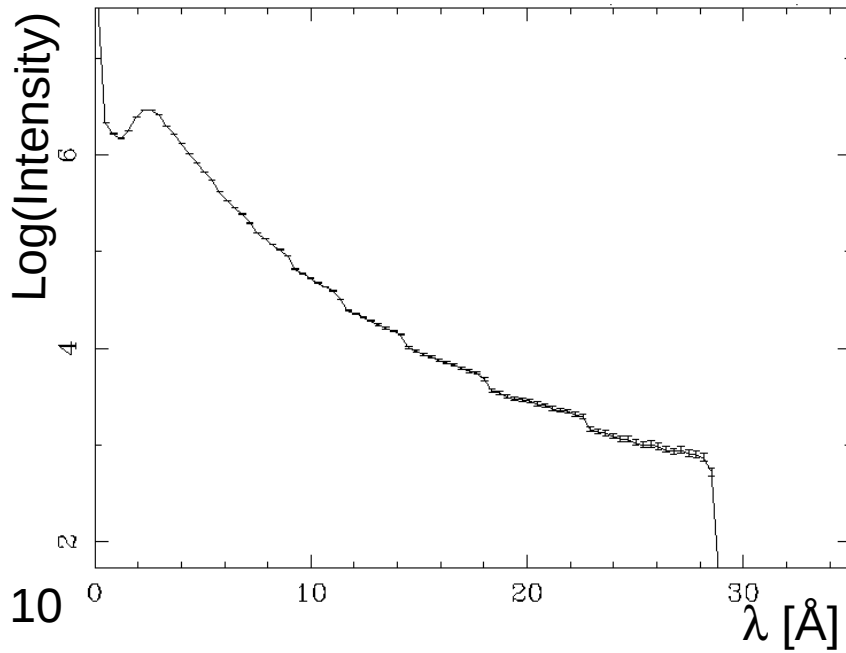
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Example3: Background along guide

- I. Neutrons generated with MCNPX
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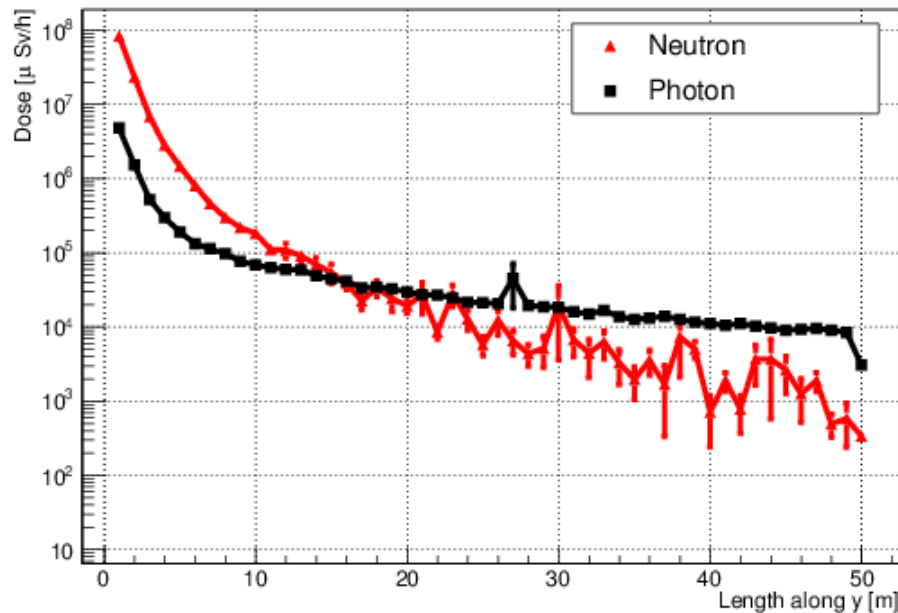


Guide end overilluminated by energetic neutrons

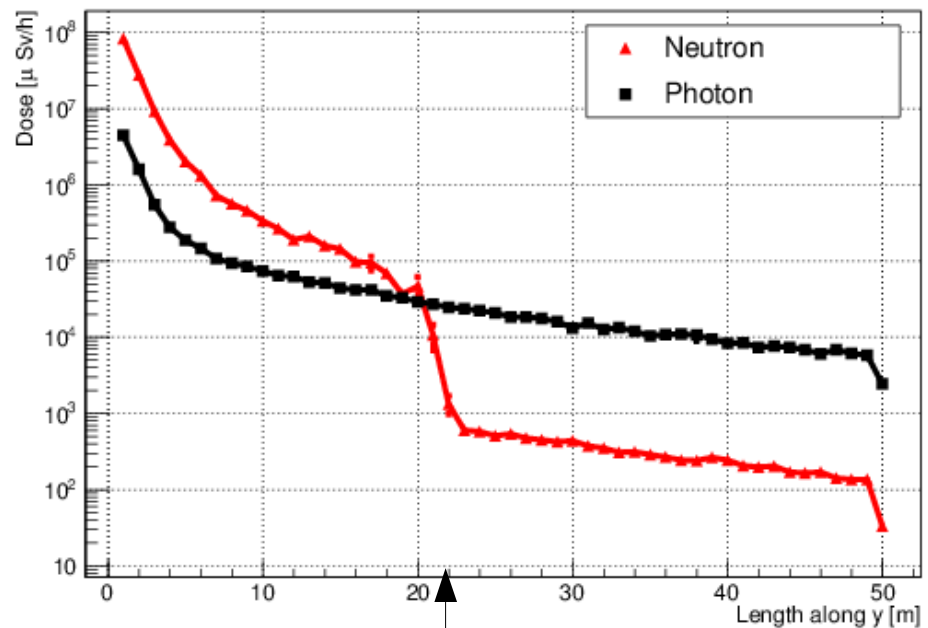


Example3: Background along guide

Straight guide



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

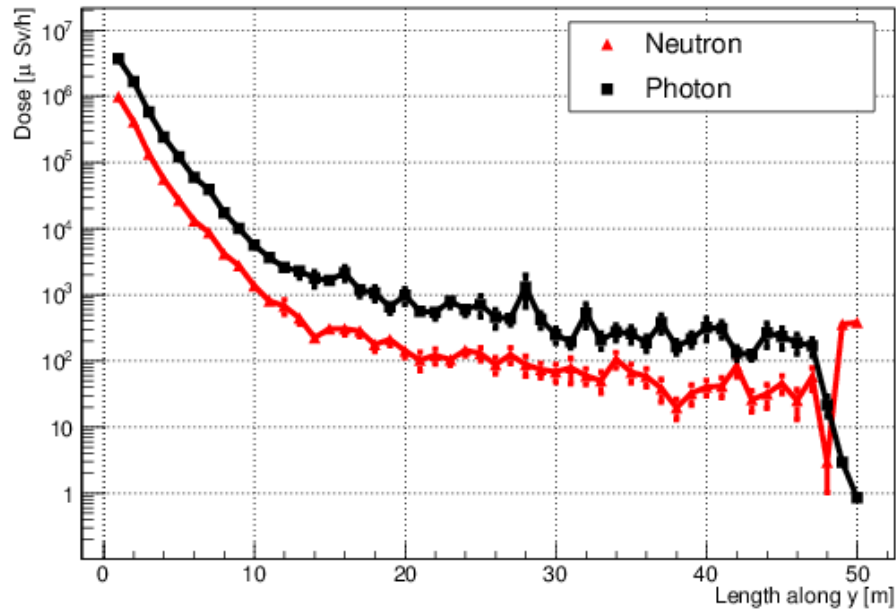


Line-of-sight lost

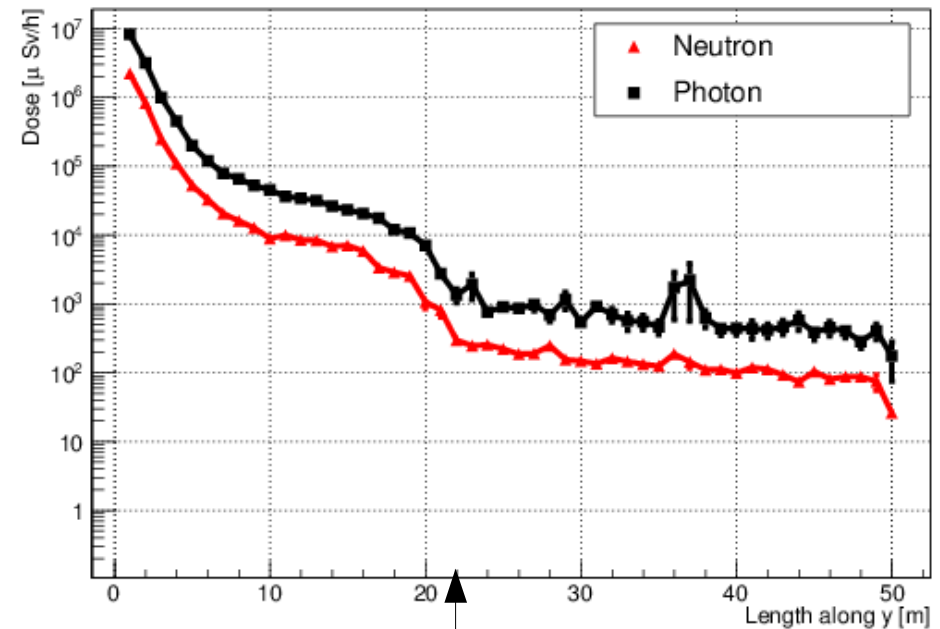
- Dose-rates, measured 5cm in the steel converted from flux according to official Swedish radiation protection procedures

Example3: Background along guide

Straight guide



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



Line-of-sight lost

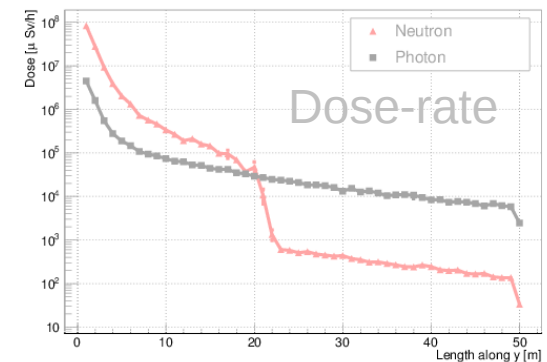
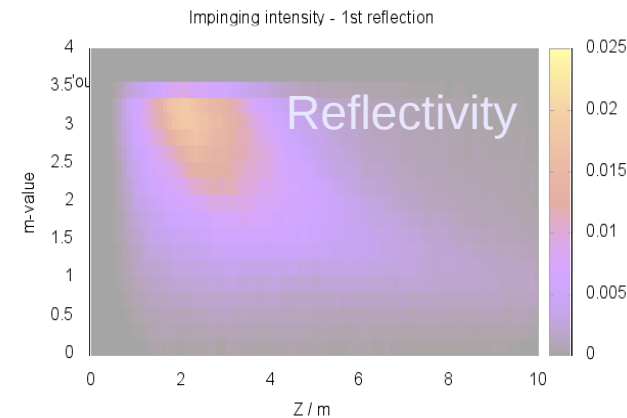
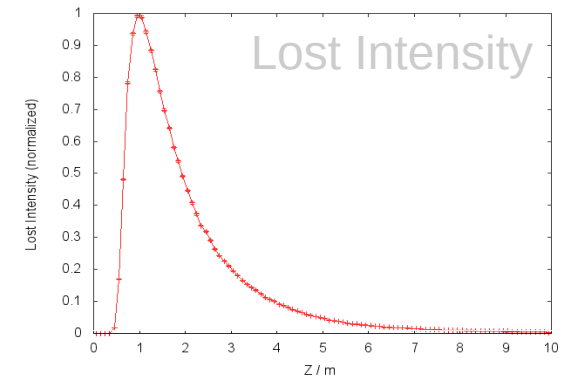
- Restricting to $\lambda \in \{0.5 \text{ \AA} - 1.0 \text{ \AA}\}$
- Photon dose-rate follows neutron dose-rate ✓

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

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

7 where Q is the scattering vector, Q_c is the critical scattering vector, R_0 is
8 the low angle reflectivity constant, W is the width of supermirror cut-off, α is
9 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

```
/*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;
```

Same as before

```
/*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:

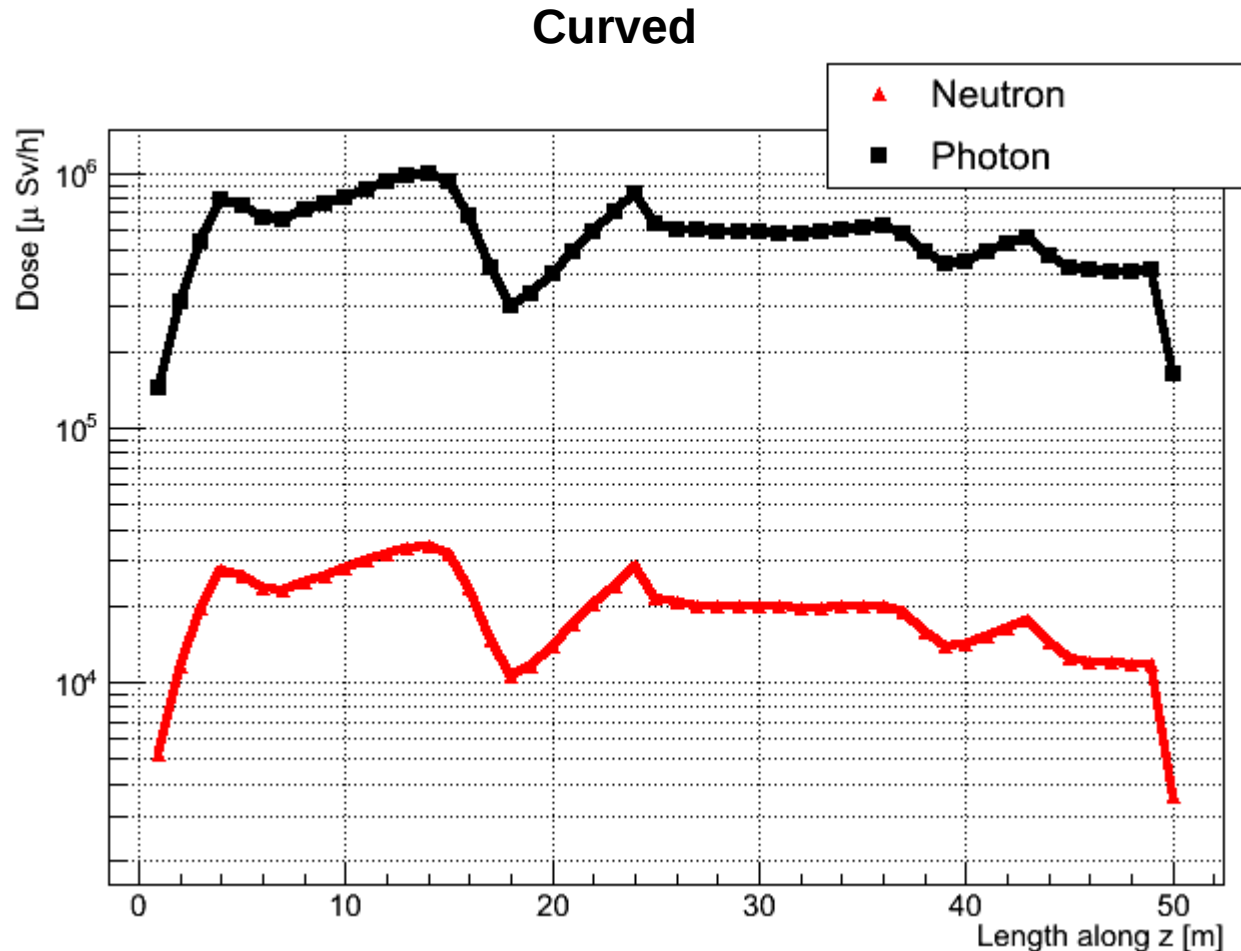


Neutron and gamma trajectories (a few example events from MCNPX → VisEd)

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

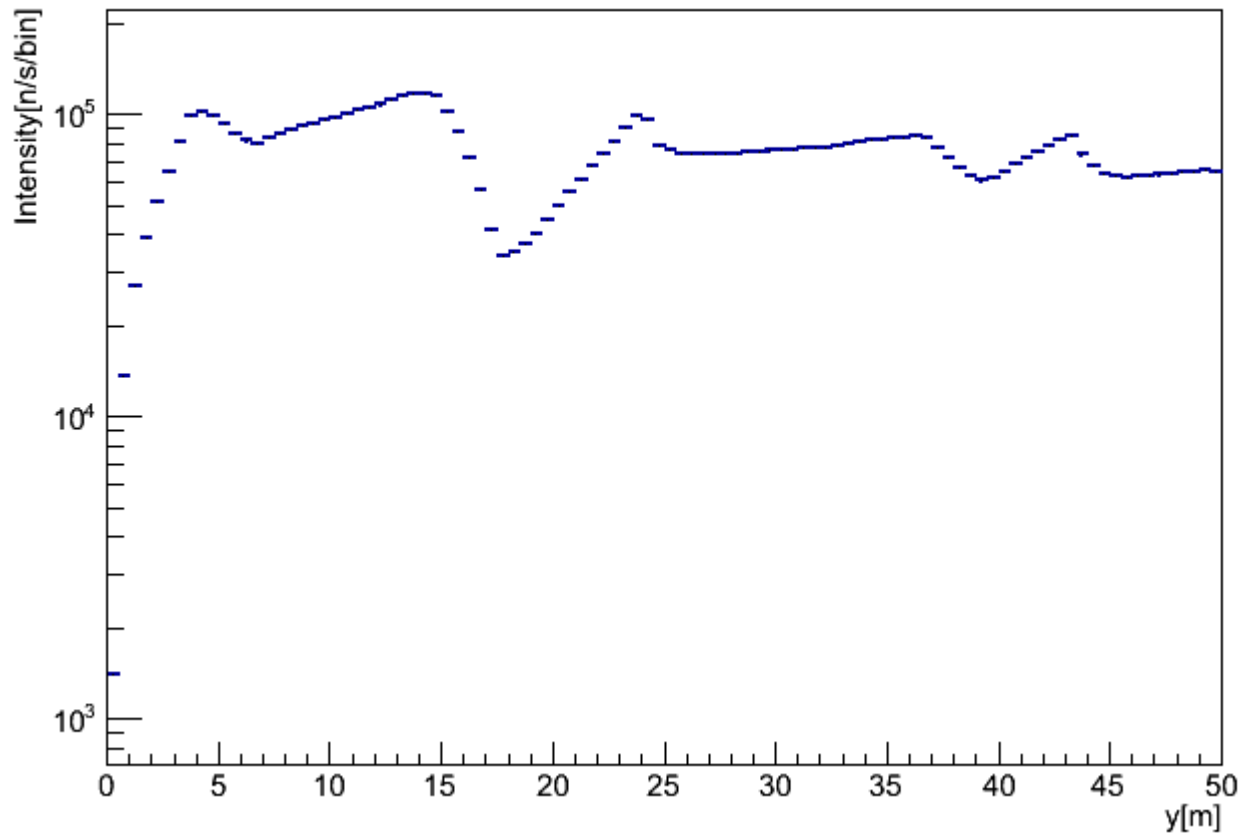


i.e. perfect match between curve structure

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 $[0.5-1]\text{\AA}$
- 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.