

Prompt gamma shielding of neutron guides from McStas Scatter Logger

Rodion Kolevatov

*Department for Neutron Material Characterization, Institutt for Energiteknikk,
Instituttveien 18, PB-40, NO-2027, Kjeller, Norway.*



Rodion.Kolevatov@ife.no

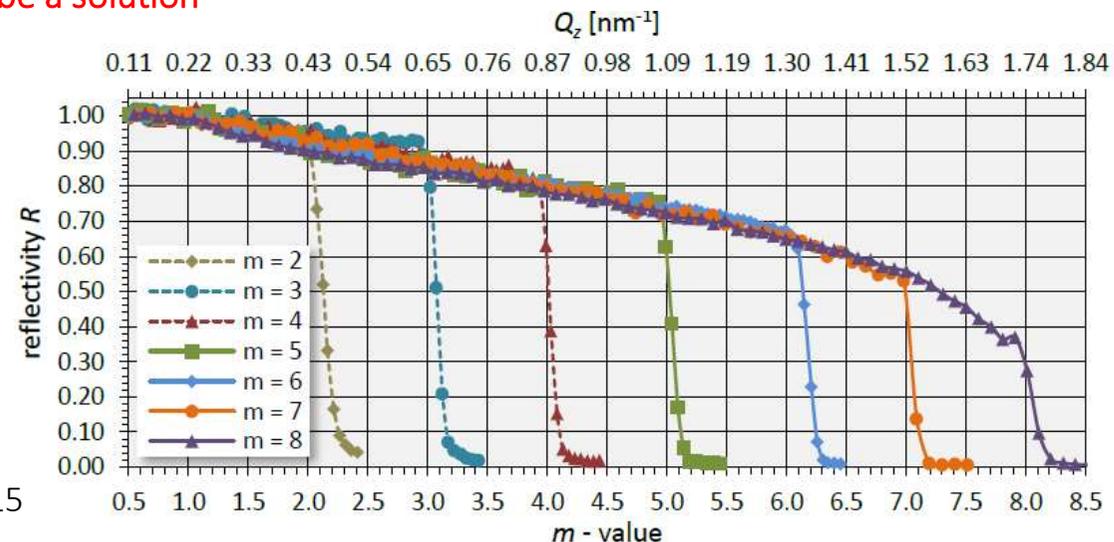
Outline

- 01 Prompt gamma radiation along neutron guides
- 02 Neutron absorption in supermirrors
- 03 Waviness effects on shielding
- 04 McStas implementation
- 05 Examples

Prompt gamma radiation accompanies neutron transport in the guides

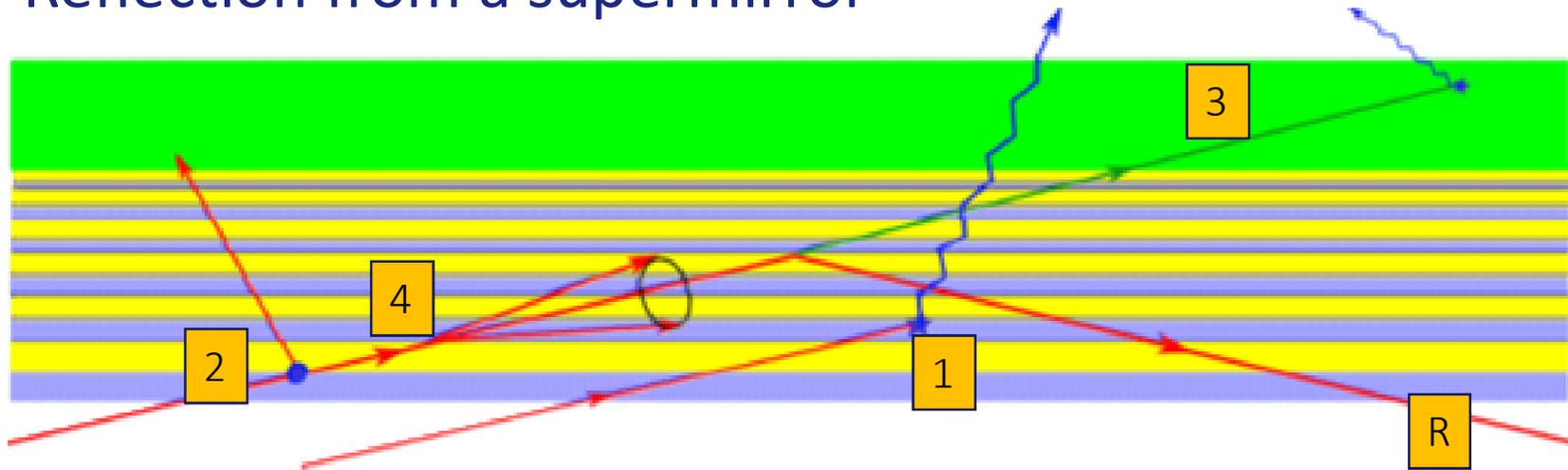
A substantial fraction of neutrons is lost at reflection during transport in the guides.

- This gives a significant contribution to the overall level of ionizing radiation
 - Up to 20% neutron capture per unreflected in high- m supermirror guide coating^{*)}
 - For a typical Ni+Ti coating composition : ~ 0.9 photons/capture with $E_\gamma > 5\text{MeV}$
 - Dominant outside line of sight/far from neutron source
- Difficult to evaluate within transport Monte-Carlo codes (for ex. MCNP, PHITS):
 - Deficiencies in implementation of supermirror physics
 - Amiguity as multilayer structure is not accounted (see later in this talk)
 - Definitions of precise geometry for the neutron optics are quite complex
 - Large execution times
- **Implementing the underlying physics** of specular reflections off the supermirrors in raytracing Monte-Carlo packages **would be a solution**



^{*)} C.Schanzer, M. Schneider, P.Böni, ECNS2015

Reflection from a supermirror

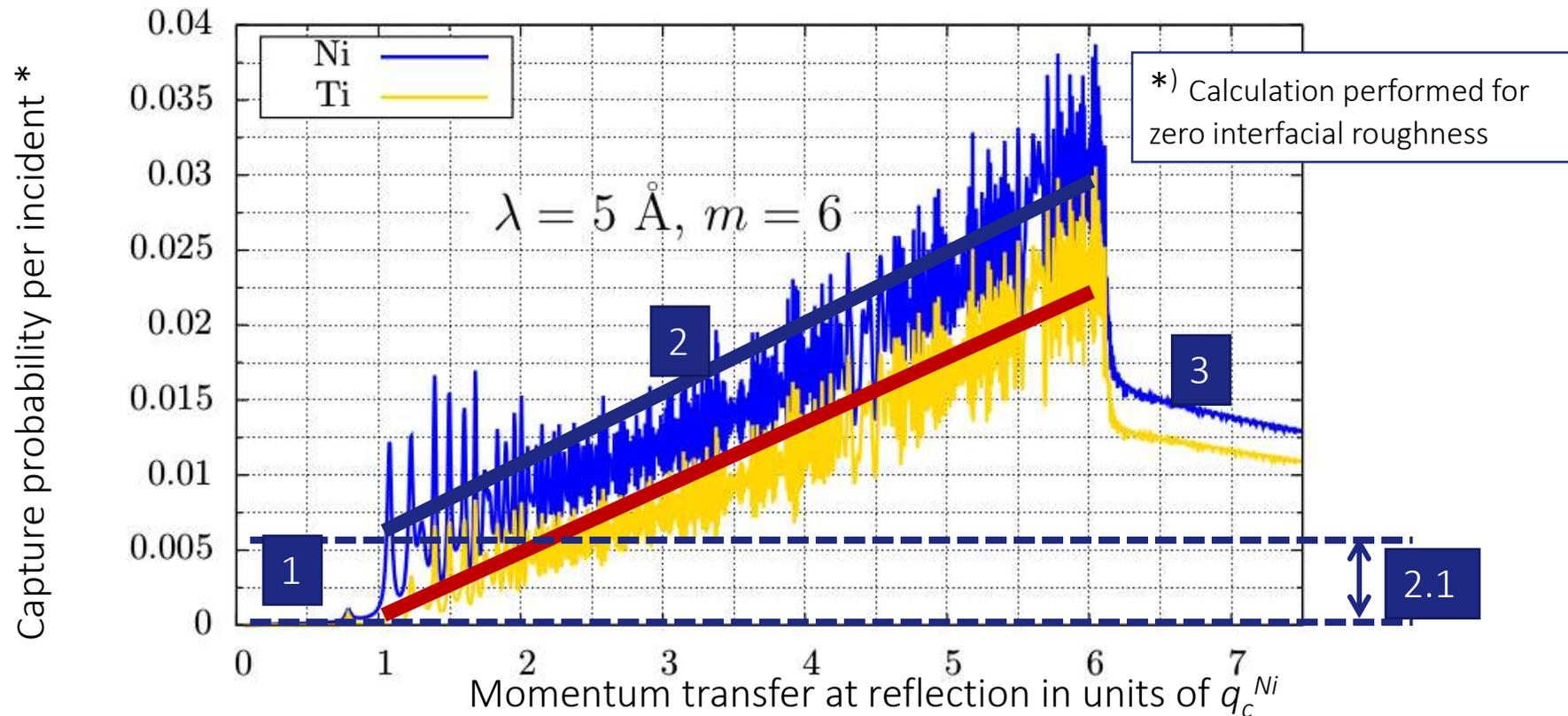


What can happen to a neutron in a Ni/Ti multilayer supermirror besides a specular reflection (R):

1. Capture ($1/v$ law: $\sigma_a \sim \frac{1}{v} \sim \lambda$)
2. Diffuse scattering in the layer bulk (isotropic, $\sigma_d = \sigma_i + \alpha(\lambda)\sigma_c$)
 - Penetrates substrate at large angle, minor capture in metal substrates
3. Transmission
 - Penetrates substrate at low angle, hence higher probability of capture in either metal or sodium float substrates.
4. Diffuse scattering on the interface roughness
5. Increase of the beam divergence due to *waviness* \Rightarrow reflectivity loss below θ_c

From a rigorous calculation:

3 distinct regimes, path length scaling



1. Little absorption per incident neutron for $q < q_c^{Ni}$.
2. Approximately linear growth for $1 < q < m q_c^{Ni}$
 1. Step in Ni absorption determined by a thickness of the outermost Ni layer
3. $1/q$ scaling above the coating cutoff (transmission for $q > m q_c^{Ni}$, path length is inverse proportional to the glancing angle)

Absorption probabilities, $q > q_c^{\text{Ni}}$

Capture probability *per incident neutron* is a universal function of $\mu \equiv q/q_c$, wavelength independent

- $1 < \mu < m$:

$$\begin{aligned} f_a^{\text{Ni}}(\mu) &= 0.005 + 0.005 \cdot (\mu - 1) \\ f_a^{\text{Mo}}(\mu) &= 0.00027 + 0.00027 \cdot (\mu - 1) \\ f_a^{\text{Ti}}(\mu) &= 0.0045 \cdot (\mu - 1) \end{aligned}$$

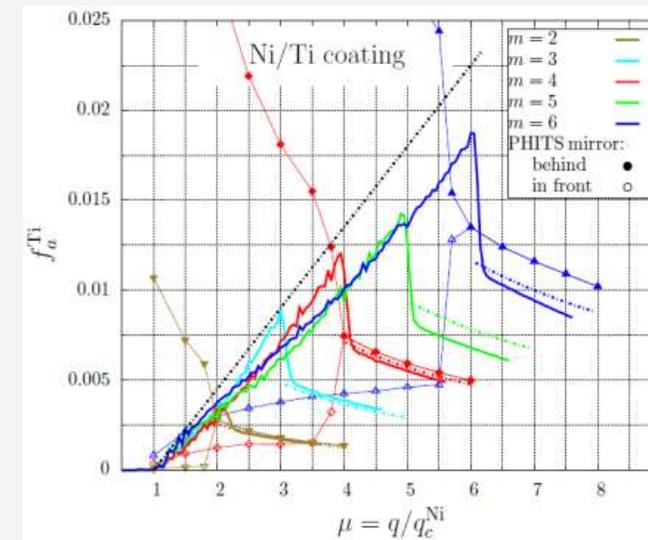
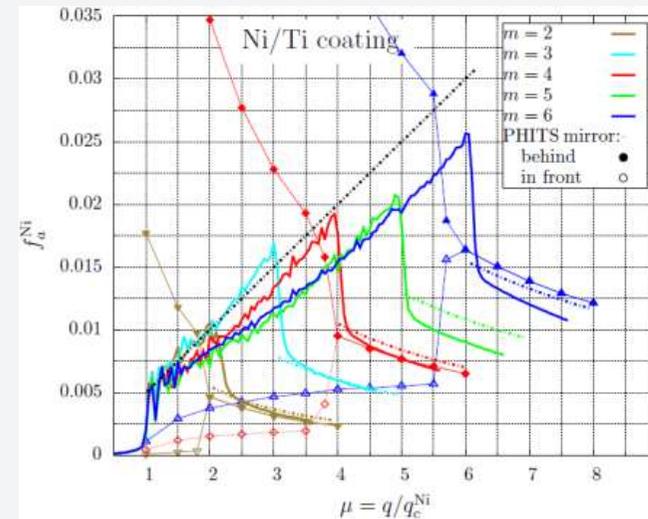
- $\mu > m$:

$$\begin{aligned} f_a^{\text{Ni}}(\mu) &= \frac{0.0025 \cdot (m + 0.1)^2}{\mu} \\ f_a^{\text{Mo}}(\mu) &= \frac{0.000135 \cdot (m + 0.1)^2}{\mu} \\ f_a^{\text{Ti}}(\mu) &= \frac{0.00225 \cdot (m - 0.9)(m + 0.1)}{\mu} \end{aligned}$$

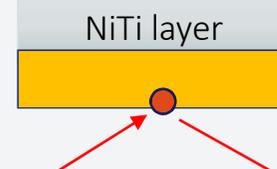
q – momentum transfer at reflection. m – supermirror coating cutoff; $q_c = 0.022 \text{ \AA}^{-1}$

- Interpretation: scales as path in the coating
- PHITS calculations of the corresponding quantities are ambiguous for $q < m \cdot q_c^{\text{Ni}}$

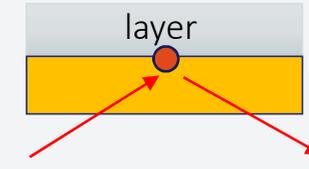
RK, P. Böni, C.Schanzer, NIM A 922 (2019) 98–107.



PHITS SM in front of



PHITS SM behind NiTi



Waviness, effects on shielding.

Physics:

- Waviness results in higher glancing angle on the average thus a certain fraction of neutrons hits coating above the cutoff and is not transported further *)
- 0.5÷1% loss/incident is compatible with waviness reported by manufacturers.

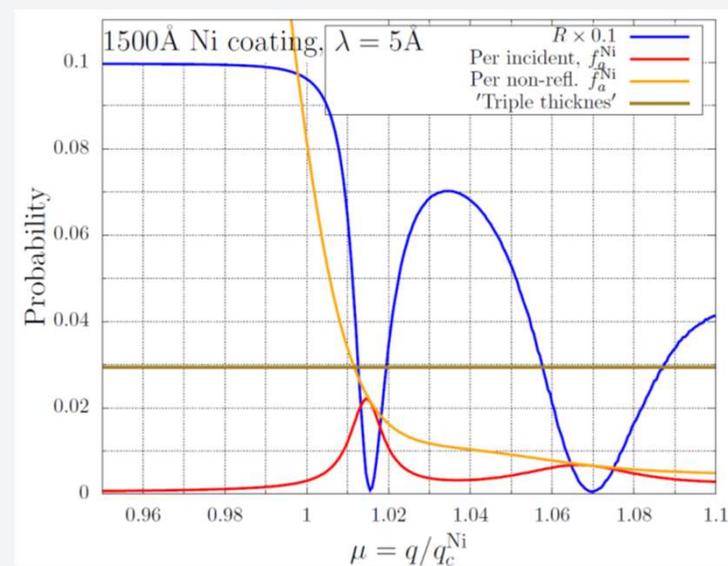
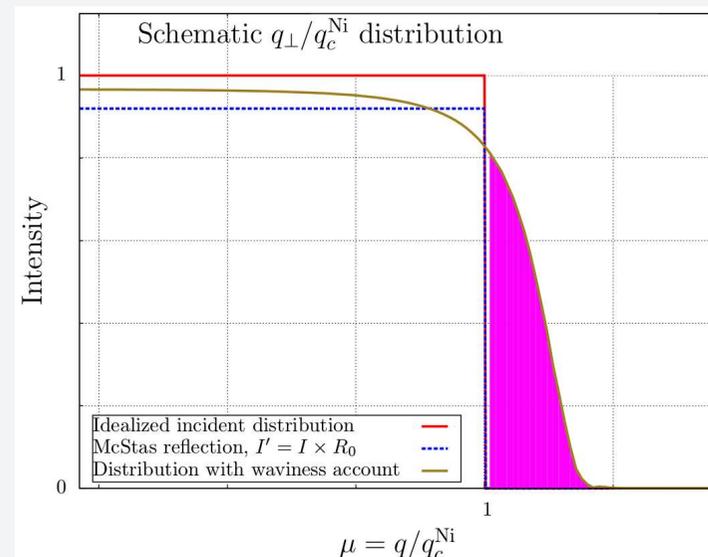
Implementation:

- Treat non-reflected neutrons with $q < q_c$ as transmitted at either first reflection minimum (single layer $m=1$) or reflection threshold (multilayer)
- A conservative estimate of *capture per non-reflected* for $m=1$ single layer (compatible with capture per non-reflected at the point of substantial drop of R):

$$P_a = \frac{\sigma_a(\lambda)}{\sigma_a(\lambda) + \sigma_d(\lambda)} (1 - e^{-6 \operatorname{Im}(K_{\min}^{\text{Ni}})d})$$

K_{\min}^{Ni} - momentum of a neutron (\perp component) hitting coating at reflection minimum while in the Ni layer; d - layer thickness.

- Typical $m=1$ coating: $\leq 1500\text{\AA}$ Ni above thin Ti layer
 - ~3% of non-reflected neutrons captured by Ni



*) Credits for explanation of the fact to the author go to Mads Bertelsen and Marton Marko.

McStas implementation

Modification of Scatter_Logger and various «Calculator» components

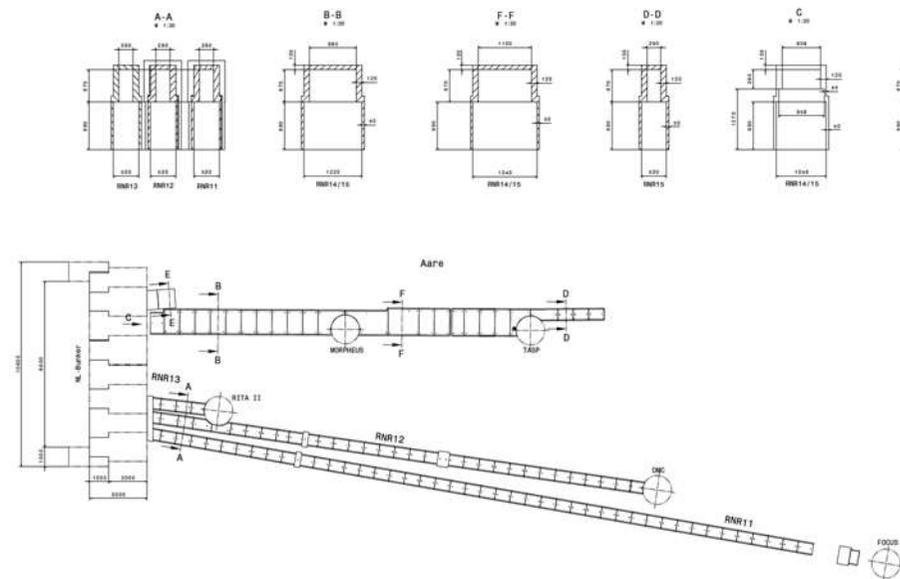
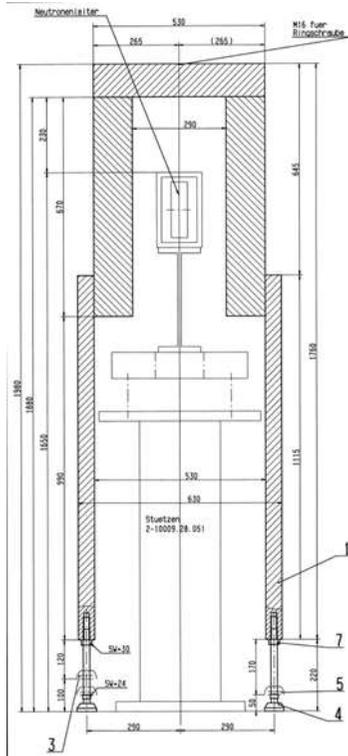
Starting point: Scatter_Logger bundle

- The Scatter_Logger component records neutron states (weight, momentum, coordinate, spin) after each reflection in the specified components of the instrument
- The Scatter_Log_Iterator iterates through the saved states and propagates pseudo-neutrons with non-reflected weight at pre-collision coordinate and momentum.

To do (actually has been done):

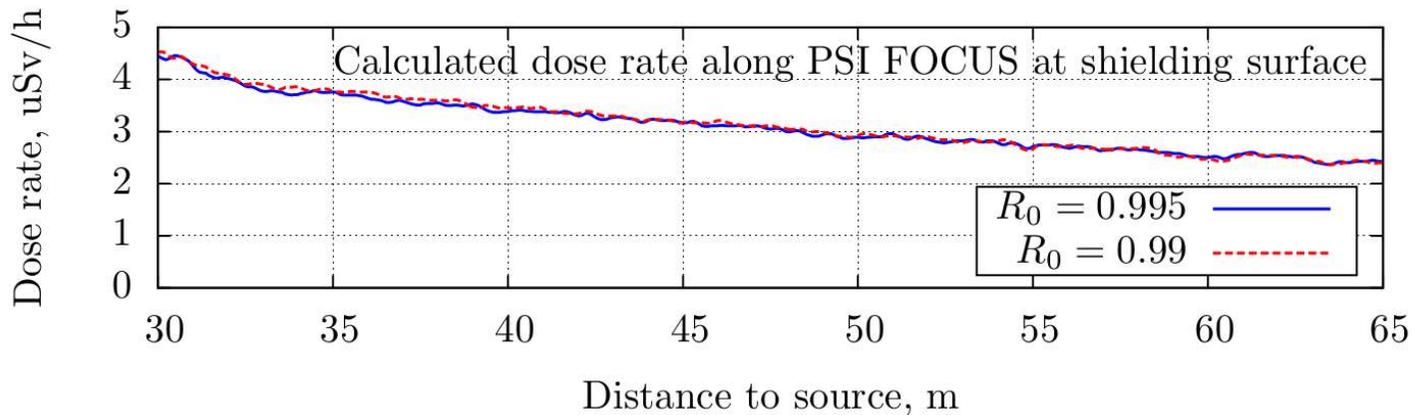
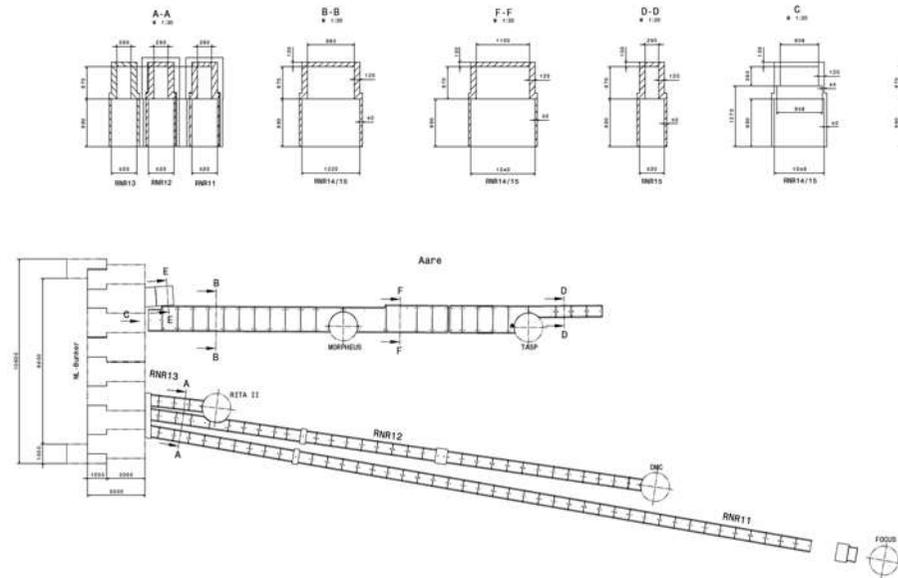
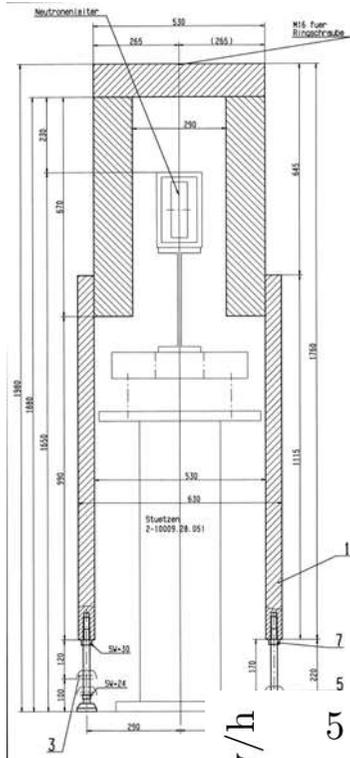
- Absorption is m-dependent. Implement recording m-value of the coating at reflection point.
- Modify Scatter_Log_Iterator to propagate pseudo-neutrons with weights corresponding to absorption in guide coating materials (3 different iterators to record capture in Ni, Ti and overall loss).
- Write a simple code to evaluate dose rate along the guide.

Benchmarking: PSI FOCUS ($m=2$)



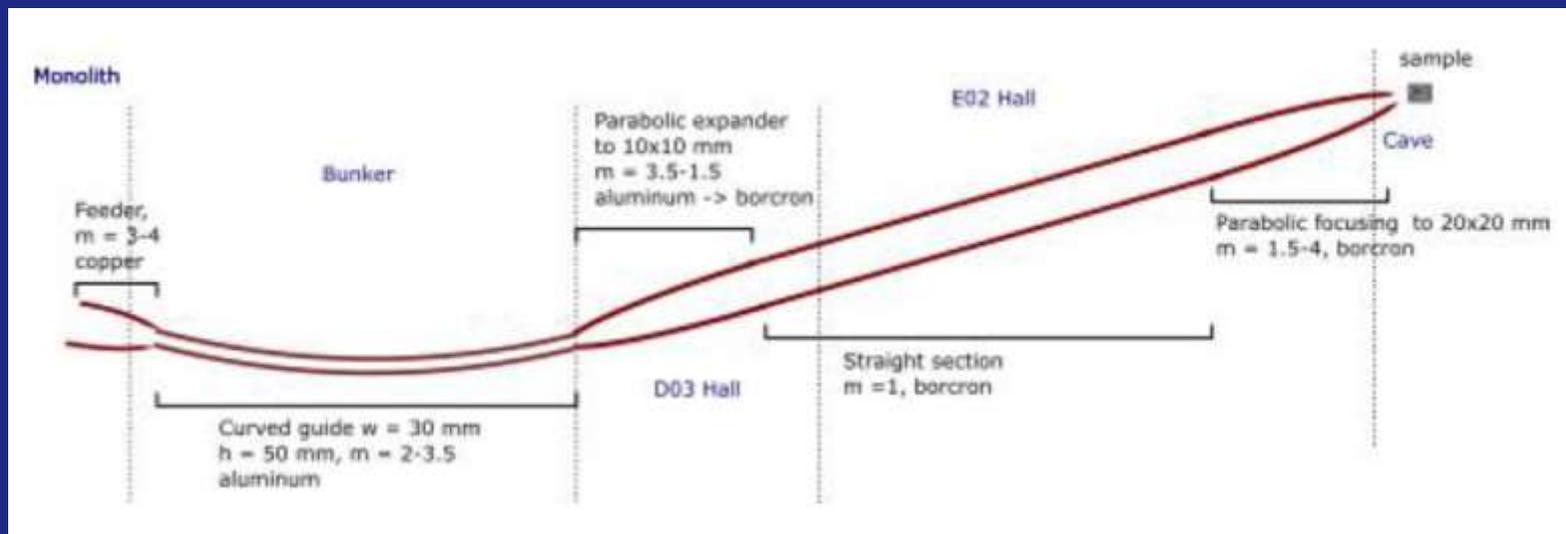
- Communicated by Uwe Filges:
 - With 120 mm steel ~ 5 $\mu\text{Sv/hr}$ at the surface,
 - Extra 50 cm concrete reduce to $<1\mu\text{Sv/hr}$ in the pathways.
 - Streaming of thermal neutron inside the steel shielding is present
 - Could result in high-E photon emission upon capture in steel

Benchmarking: PSI FOCUS ($m=2$)



Usage example (defocusing section of the ESS BIFROST instrument)

Modifying instrument file and adding «Calculator» components



Logging

- Surround a part of the instrument of interest with LoggerStart and Stop.
- Specify a name of the logger stop (needed to have a possibility for more than one logger in a file)

```

alpha=3.100000,W=0.003000,
mleft = 3.000000, mright = 3.500000,
mtop = 2.500000,mbottom =2.500000)
AT (7.57345916228e-10,0,0.500 + u + 6e-5) RELATIVE PREVIOUS // curved_guide_34_0
ROTATED (0,benderAngle,0) RELATIVE PREVIOUS // curved_guide_34_0

COMPONENT EndOfelement_4= Arm()
AT (7.57345916228e-10,0,0.495689132 + u) RELATIVE PREVIOUS // curved_guide_35_0

COMPONENT Div2d_AfterBender = Divergence_monitor(
  nh = 200, nv = 200, filename = "Div2d_AfterBender.dat", xwidth = 0.1, restore_neutron=1,
  yheight = 0.1, maxdiv_h = 2.5, maxdiv_v = 1.5)
AT (0, 0,u) RELATIVE PREVIOUS

/***** Start of scatter logger. Logging scatterings and absorption in the guide system. *****/
COMPONENT log_P_start=Shielding_logger()
AT (0,0,0) RELATIVE PREVIOUS
EXTEND
%{
#ifdef scatter_logger_stop
#undef scatter_logger_stop
#endif
#define scatter_logger_stop log_P_start
%}

COMPONENT elliptical_guide_gravity3= Elliptic_guide_gravity_custom(
l=24.928800, linxw=3.709727, linyh=4.423828, loutxw=28.638527, loutyh=29.352628,
xwidth = 0.060000, yheight = 0.090000, dimensionsAt="mid",
R0=0.990000, Qc=0.021700, alpha=3.100000, mvaluesright = mValues3horizontalS, mvaluesleft = mValues3horizontalS,mvalue
AT (0,0, u) RELATIVE EndOfelement_4
ROTATED (0,0,0) RELATIVE EndOfelement_4

COMPONENT EndOfelement_3= Arm()
AT (0,0,24.928800+u) RELATIVE PREVIOUS

/*Stop of scatter logger. Record scatterings in what is between start and stop, that is, parabolic feeder.*/
COMPONENT log_P_stop=Shielding_logger_stop(logger=log_P_start)
AT (0,0,0) RELATIVE PREVIOUS

```

Line: 1406 of 1791 total, Column: 0

Iterating

- Iterators to process saved states
- Monitor_nD within iterator start and stop to record coordinate along the guide
 - Can record other quantities as well, e.g. divergence of neutrons absorbed in particular coating materials.

```

Edit: BifrostV4_1_Shielding.instr
File Edit Search View Insert

COMPONENT log_P_stop=Shielding_logger_stop(logger=log_P_start)
AT (0,0,0) RELATIVE PREVIOUS

|

/*===== ITERATOR SECTION. PROCESSING STORED EVENTS =====*/
/* Insert this into McStas instrument file to do the costs evaluation */
COMPONENT arm_iter_P1_start=Arm()
AT(0,0,0) RELATIVE ESS_source

COMPONENT iter_P1_start = Shielding_log_iterator_Ni_new()
AT (0,0,0) RELATIVE ESS_source //ABSOLUTE
EXTEND
%{
#kdef scatter_iterator_stop
#undef scatter_iterator_stop
#endf
#define scatter_iterator_stop iter_P1_start
%}
JUMP arm_iter_P1_stop WHEN(optics_not_hit)

/*Monitoring the tracks stored by the scatter logger*/
/*Putting dummy arm to register all neutrons to ensure that monitors_nD with shape "previous" will process them */
COMPONENT arm_iter_P1_dummy=Arm ()
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT mndP01=Monitor_nD (
restore_neutron=1, zmin=25.0,
zmax=50,
bins=250, options="previous no slit z ", filename="NiCapture.dat")
AT(0,0,0) RELATIVE ESS_source //RELATIVE source

COMPONENT arm_iter_P1_stop=Arm()
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT iter_P1_stop = Shielding_log_iterator_stop(iterator=iter_P1_start)
AT(0,0,0) RELATIVE ESS_source

/*Moving again to the reference point of iterator start
when there are still some tracks stored to perform iterations with,
checked by the function MC_GETPAR */
COMPONENT a11i = Arm()
AT (0,0,0) RELATIVE EndOfelement_3
JUMP arm_iter_P1_start WHEN(MC_GETPAR(iter_P1_stop,loop))

/*===== END OF PROCESSING. END OF ITERATOR SECTION =====*/

/*===== ITERATOR SECTION2. PROCESSING STORED EVENTS =====*/

Line: 1406 of 1791 total, Column: 0

```

Iterating

- Same buffer of the saved states has to be processed for 3 times for Ni capture, Ti capture and total loss.
- In the last of the 3 iterators the variable last has to be set to **last=1** to clear memory used for the saved states.

```

Edit: BifrostV4_1_Shielding.instr
File Edit Search View Insert

/* ***** END OF PROCESSING. END OF ITERATOR2 SECTION ***** */
/* ***** ITERATOR SECTION3. PROCESSING STORED EVENTS ***** */
/* Insert this into McStas instrument file to do the costs evaluation */
COMPONENT arm_iter_P3_start=Arm()
AT(0,0,0) RELATIVE ESS_source

COMPONENT iter_P3_start = Shielding_log_iterator_total()
AT (0,0,0) RELATIVE ESS_source //ABSOLUTE
EXTEND
%{
#ifdef scatter_iterator_stop
#undef scatter_iterator_stop
#endif
#define scatter_iterator_stop iter_P3_start
%}
JUMP arm_iter_P3_stop WHEN(optics_not_hit)

/*Monitoring the tracks stored by the scatter logger*/
/*Putting dummy arm to register all neutrons to ensure that monitors_nD with shape "previous" will process them */
COMPONENT arm_iter_P3_dummy=Arm ()
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT mndP03=Monitor_nD (
restore_neutron=1, zmin=25.0,
zmax=50.0,
bins=250, options="previous no slit z ", filename="TotalCapture.dat")
AT(0,0,0) RELATIVE ESS_source //RELATIVE source

COMPONENT arm_iter_P3_stop=Arm()
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT iter_P3_stop = Shielding_log_iterator_stop(iterator=iter_P3_start, last=1)
AT(0,0,0) RELATIVE ESS_source

/*Moving again to the reference point of iterator start
when there are still some tracks stored to perform iterations with,
checked by the function MC_GETPAR */
COMPONENT a13i = Arm()
AT (0,0,0) RELATIVE EndOfelement_3
JUMP arm_iter_P3_start WHEN(MC_GETPAR(iter_P3_stop,loop))

/* ***** END OF PROCESSING. END OF ITERATOR3 SECTION ***** */

COMPONENT Beamstop = Beamstop(
)
AT (0, 0, 0.01) RELATIVE EndOfelement_3

COMPONENT Div2d_BeforeStraight = Divergence_monitor(
nh = 200, nv = 200, filename = "Div2d_BeforeStraight.dat", xwidth = 0.1, restore_neutron=1,
yheight = 0.1, maxdiv h = 1, maxdiv v = 1)

```

Line: 1495 of 1791 total, Column: 0

Calculating

- *Shielding_calculator* component outputs shielding thickness for given dose outside
- *Dose_calculator* outputs dose rate outside shielding of fixed thickness
- Input used: text files generated by Monitor_nD components recording capture along the guide
 - File names need to be specified as arguments
 - Can arrange a separate “instrument” for shielding calculation which reads previously calculated capture and loss rates.
- Components implement
 - Analytical formula for dose rate attenuation
 - table values for the capture γ spectra in Ni, Ti and borosilicate (19 E groups)
 - Linear attenuation and buildup factors of typical shielding materials
 - Flux to dose factors

```

Edit: JustShielding.instr
File Edit Search View Insert

//strcat(temp,mcdirname);
//strcat(temp,separator);
strcat(temp,".");
strcat(temp,separator);
strcat(temp,diname);
strcat(temp,separator);
//strcat(temp,"/home/rodionk/SHIELDING_TASKFORCE/ESS_SHIELDING/C-SPEC/NO_CHOPPERS_COMMONSOLUTIONS.");
strcat(nifile,temp);
strcat(nifile,nidata);
strcat(tifile,temp);
strcat(tifile,tidata);
strcat(totfile,temp);
strcat(totfile,totdata);
printf("%s\n%s\n%s\n",nifile,tifile,totfile);
%}

TRACE

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

COMPONENT ESS_Source = ESS_butterfly(sector="W",beamline=3,Lmin=0.1,Lmax=100,dist=1.9,cold_frac=0.5,yheight=0.03,foct)
AT (0,0,0) RELATIVE Origin

/*Calculating shielding requirements to assure 5 microSivert/hour at the outer shielding surface*/
/*Inner space in the shieling is 30 cm wide, gamma radiation and lost neutron information is taken from the files of the correspondin
/*Number of bins in the monitors should match each other*/
COMPONENT SCalc=Shielding_calculator(MaxRate=1.0,Innerspace=0.5,
NiCaptureFile=nifile,TiCaptureFile=tifile,TotalCaptureFile=totfile,OutputFile="Shielding.dat")
AT (0,0,0) RELATIVE PREVIOUS

/*Calculating dose rates at the surface of lateral shielding along the guide. 12 cm steel and 50 cm concrete.*/
/*Inner space in the shielding is assumed 30 cm wide, the guide is in the middle of the shielding housing.*/
COMPONENT DoseFe=Dose_calculator(Innerspace=0.4,Thickness=0.2,
Material="Fe",NiCaptureFile=nifile,TiCaptureFile=tifile,TotalCaptureFile=totfile,OutputFile="DoseFe.dat")
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT DoseConc=Dose_calculator(Innerspace=0.4,Thickness=0.6,
Material="Concrete",NiCaptureFile=nifile,TiCaptureFile=tifile,TotalCaptureFile=totfile,OutputFile="DoseConc.dat")
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT DoseStandard=Dose_calculator(Innerspace=0.4,Thickness=0.4,
Material="Concrete",SteelTubing="yes",
TubingThickness=0.1,NiCaptureFile=nifile,TiCaptureFile=tifile,TotalCaptureFile=totfile,OutputFile="DoseConcTubing.dat")
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT Dose5=Dose_calculator(Innerspace=0.4,Thickness=0.6,
Material="Concrete",SteelTubing="yes",
TubingThickness=0.05,NiCaptureFile=nifile,TiCaptureFile=tifile,TotalCaptureFile=totfile,OutputFile="DoseConcTubing5.dat")
AT (0,0,0) RELATIVE PREVIOUS

END

Line: 82 of 93 total, Column: 0

```

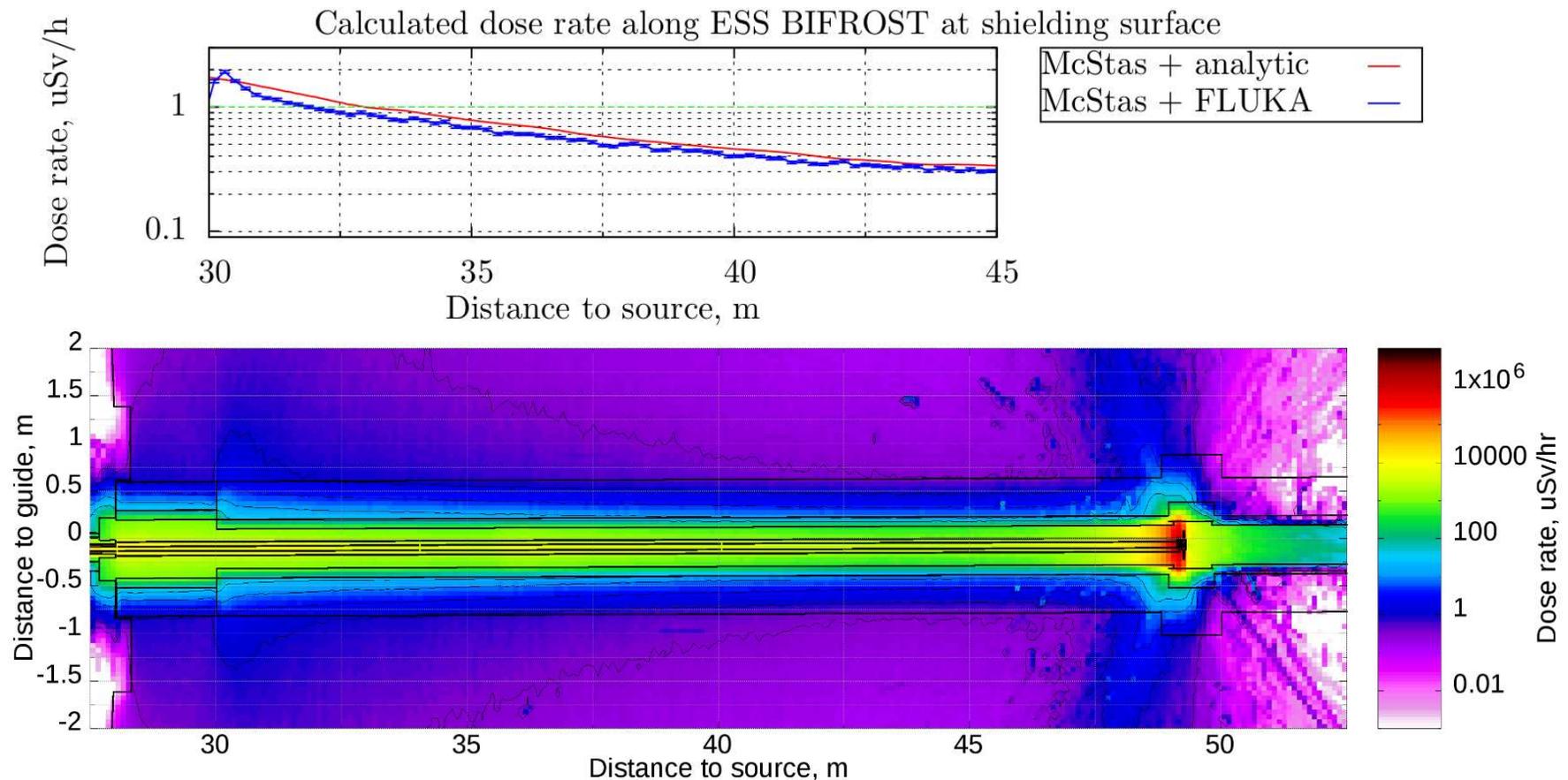
FLUKA simulation of ESS BIFROST guide and beam shutter

Lateral shielding is composed of 10 cm steel followed by 40 cm concrete.

Two custom FLUKA source routines:

- Output of Shielding iterators
- McStas generated mcpl file for neutrons hitting the shutter

In a particular case of BIFROST, streaming of fast neutrons from the source is a minor source of radiation. Otherwise – need the third source routine.



Final remarks

- The Shielding Suite provides reliable estimates of dose rates along the neutron guides.
- Very fast: analytic evaluation takes several minutes on a laptop (including running instrument file in McStas).
- Currently available from author on request.
- If interested, please stop by the poster at the first poster session at ECNS.
- The content of the talk will hopefully be published as a paper in the proceedings of the ECNS. Otherwise see ESS report number 0511500.
[https://indico.ess.lu.se/event/1183/attachments/8589/12941/ESS-0511500 -
_Prompt_gamma_shielding_for_the_neutron_guides_at_the_ESS.pdf](https://indico.ess.lu.se/event/1183/attachments/8589/12941/ESS-0511500_-_Prompt_gamma_shielding_for_the_neutron_guides_at_the_ESS.pdf)

Thanks to:

Peter Böni, Marton Marko, Erik Knudsen, Uwe Filges, Mads Bertelsen, Kim Lefmann, members of BIFROST and HEIMDAL teams.

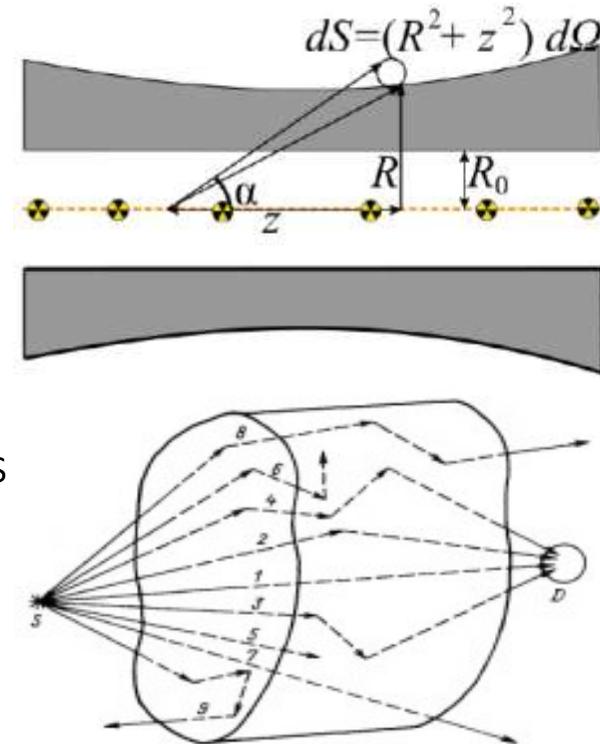
Backup files

Implementation details:

- Customize McStas components to set **variable for m-value** at reflection point:
 - *Guide_custom, Guide_curved_custom* (to replace *Bender* in shielding calculations, has same syntax), *Elliptic_guide_gravity_custom, Guide_chanelled_custom*
- Make **McStas Scatter Logger** by E. Knudsen et al record m-value at reflection → *Shielding_logger* component
 - Possible to have several independent loggers along the instrument.
 - Minor bug correction to handle some rare cases (e.g. neutron went through with no reflections)
- **Implement coating capture probability** in Scatter Log Iterator:
 - *Shielding_log_iteratorNi, Shielding_log_iteratorTi, Shielding_log_iterator_total* iterate through the unreflected states returning corresponding weights for capture
 - Processing neutrons entering iterators allows a straightforward construction of source terms for Monte-Carlo transport codes.
- Table values for the capture γ spectra in Ni, Ti and borosilicate, attenuation and buildup factors of typical shielding materials are implemented in *Shielding_calculator* component (calculates shielding thickness for given dose outside) and *Dose_calculator* (dose rate outside shielding of fixed thickness)

Dose rate from gamma

- Neutrons captured in the guide walls give extended source of radiation: $I(E, z)$ (McStas)
- Photon spectrum: 19 groups from IAEA data
- Contribution of *direct* photons decreases exponentially with shielding thickness $e^{-\mu(E)d(z)}$ (NIST data for μ)
- Contribution of *scattered photons* and secondaries – “*dose buildup*”: $B_{\text{dose}}(E, \mu d)$ (Mashkovich)
- Biological effect varies with γ energy. Flux to dose rate conversion: $K(E)$ (ESS-19931)



$$\dot{H}(R, z) = \frac{1}{4\pi} \int dz dE K(E) I(E, z) B_{\text{dose}}(E, \mu d(z)) \frac{1}{(R^2 + z^2)} e^{-\mu(E)d(z)}$$

$$d(z) = \frac{(R - R_0)\sqrt{R^2 + z^2}}{R}$$