International Collaboration on Advanced
Neutron Sources (ICANS XXIII)

Detailed supermirror physics in MCNP6

ESS-Bilbao

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Introduction

Introduction

Shielding in neutron beamlines is a complex problem for several reasons, such as the long distance streaming, but in particular, the neutron reflection in the guides is a phenomenom that is typically not implemented in Monte Carlo codes. Because of this, calculation of shielding in the guides must rely on some coupling with guide-specific codes such as McStas, or some assumptions on the neutron transport. Thus, having this physics implemented in Monte Carlo group is of interest.

Antecedents

PHITS features supermirror physics starting from version 2.12. Geant4 does not feature this physics, and D. Di Julio has performed some work regarding its implementation. In the MCNP camp, F.X. Gallmeier created a patch for MCNPX that allows the user to include reflecting surfaces calculated with the same empirical equation used in McStas. However, MCNPX is being superseded by MCNP6, which backports features from MCNP5 such as FMESH mesh tally, as well as other new improvements.

Code porting

Verification and validation

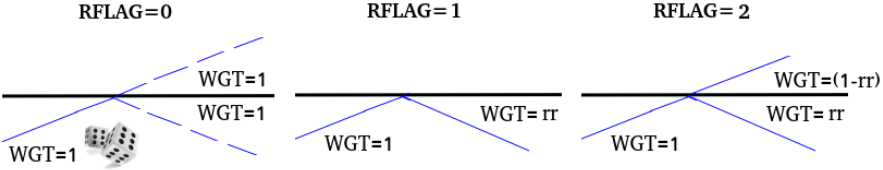
In October 2018, the port to MCNP6 was completed, and we verified the results in a number of tests, in the context of the SINE2020 project. In particular, we benched it againts previous MCNPX implementation. The results fall well between the margin of variance between both codes.

Tally	Distance m	MCNPX Result	MCNP6 Result	% Diff
12	0.5	2.94E-1	2.87E-1	2.59%
22	1.5	1.13E-1	1.10E-1	2.52%
32	2	6.09E-2	6.08E-2	0.13%
42	3	4.74E-2	4.66E-2	1.85%
52	7.5	1.88E-2	1.81E-2	3.76%
62	9.5	1.43E-2	1.36E-2	4.77%
72	25	6.21E-3	5.96E-3	4.70%
82	45	4.50E-3	4.30E-3	5.21%
92	66	3.82E-3	3.64E-3	5.70%

Enhancements to the code

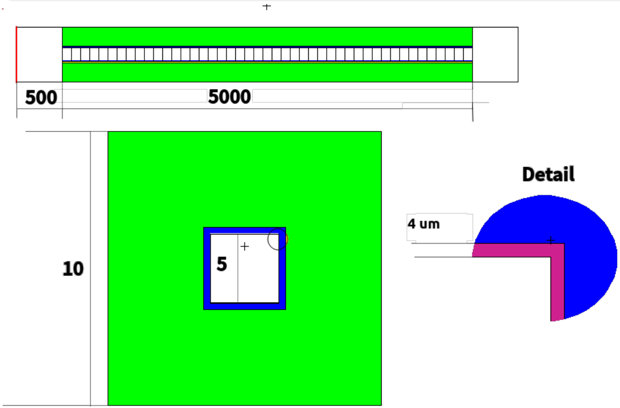
Reflection mode: In-guide only and splitting

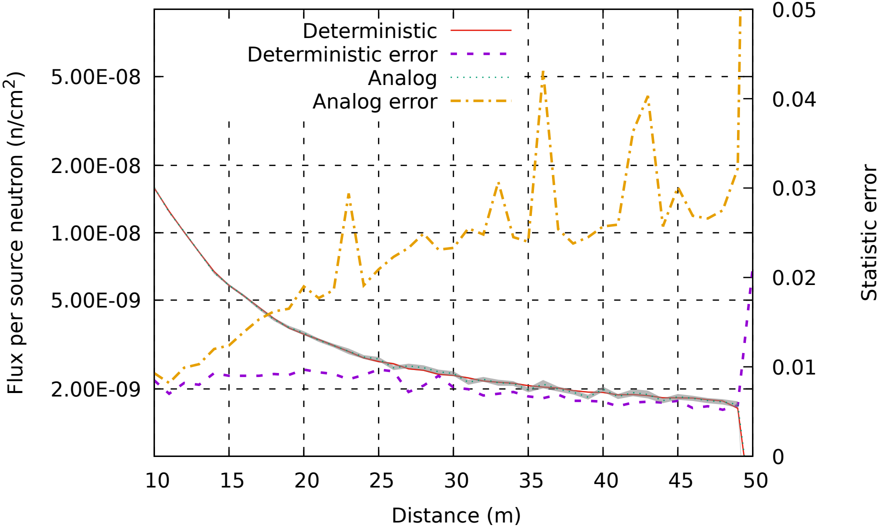
Once the port was done, we focused on implementing improvements that allow for more powerful simulations. The first one is enabling the possibility of three different reflection modes: The first one is the one previously implemented, the second one can be seen similar to a McStas simulation (discarding the lost neutrons), and the third one splits the neutrons in transmitted and reflected parts. Notice that only the first mode implies a RANG() call, so the other two are, effectively, deterministic transport.



Benefits of the splitting at mirrors

Splitting the particle into reflected and transmitted part smoothes the distribution of the particles. Reflected particles progressively lose some weight down the guide, while transmitted particles, specially in scenarios where the reflectivity is close to 1, are much better sampled. This enables better calculation of neutron flux, and generated gamma.




Deterministic
Deterministic error
Analog
Analog error
Flux per source neutron (n/cm^2)
5.00E-08
2.00E-08
1.00E-08
5.00E-09
2.00E-09
0.05
0.04
0.03
0.02
0.01
0
Statistic error
10
15
20
25
30
35
40
45
50
Distance (m)

Enhancements to the code (II)

DXT spheres

Detectors and Direct Transport Spheres (DXT) are incompatible with any kind of reflecting surface, as the MCNP sternly warns. The reason is that it is not possible to calculate the contribution from a collision or source (primary or secondary) through a reflection, but if the reflected particle enters the sphere, it will still get killed.

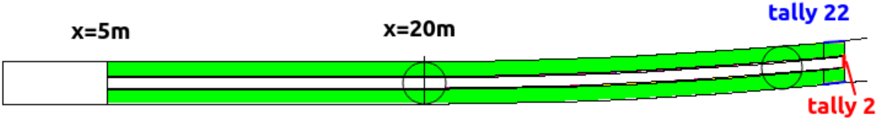
Solution to this problem

Our solution to the problem is to make the DXT “fair” by not killing the particles whose contribution it could not calculate. This is done by setting up a flag that makes the particle invisible to DXT, raising it in a reflection event, and lowering it in a collision. The code for making the sphere invisible to it is actually already present in the function dist_dxtran_sphere().

DXT sphere testbench

Description

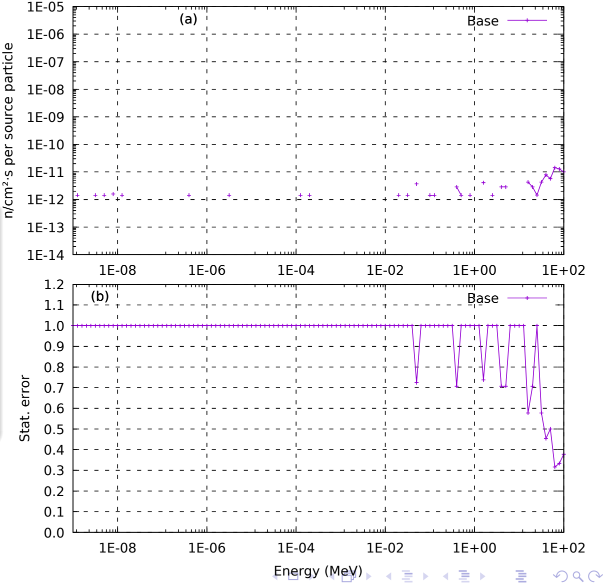
We tested the new DXT code in different configurations, including double and nested DXT to check for cross-talking. This allows us to see the effects of the DXT and the mirror card, in stock and patched configurations. The source is a 0.1 meV to 100 MeV with homogeneous lethargy distribution, in a 4 degrees cone. a 15m straight guide is followed by a 2km radius curve for another 20m. Tally 2 checks the flux at the end of the guide, and tally 22 checks the neutron leak in the final meter.



DXT results(End of guide)

Effects of mirror card and DXT

First set of results is the base case (no DXT and no mirror), only mirror card, only DXT, 'stock' DXT with mirror, and new DXT with mirrors. Runtime is roughly constant at 10.000 minutes-core in order to have more comparable results.



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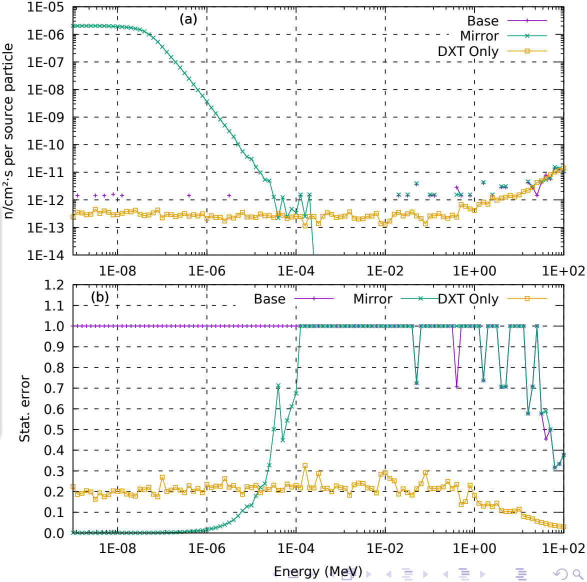

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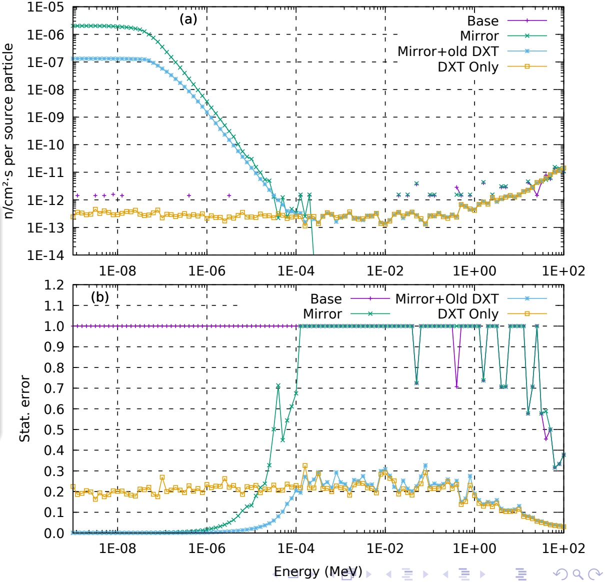

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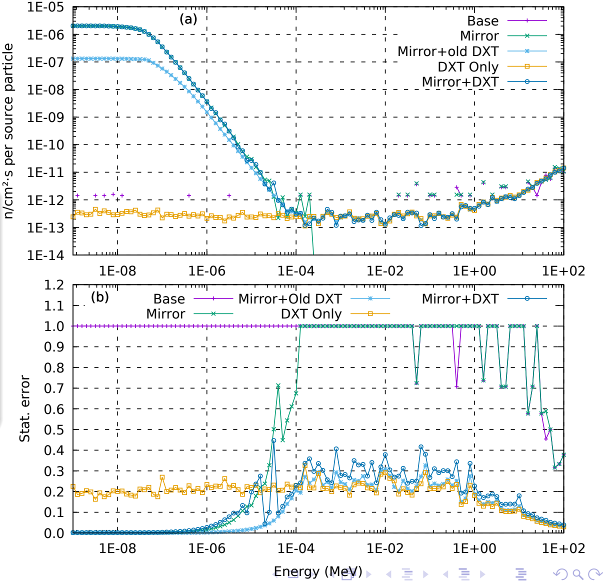

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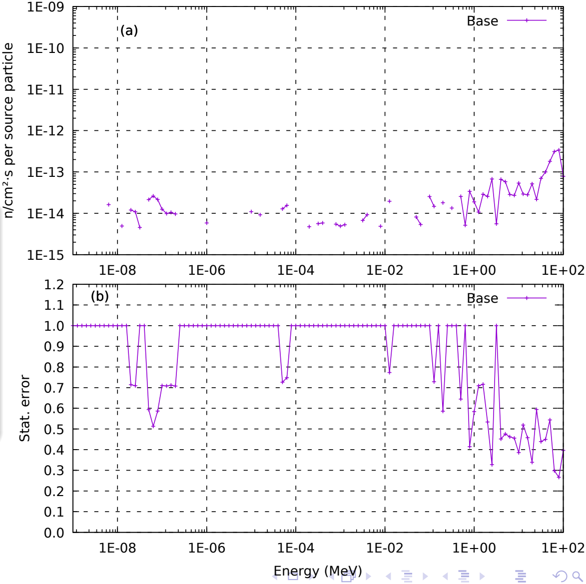

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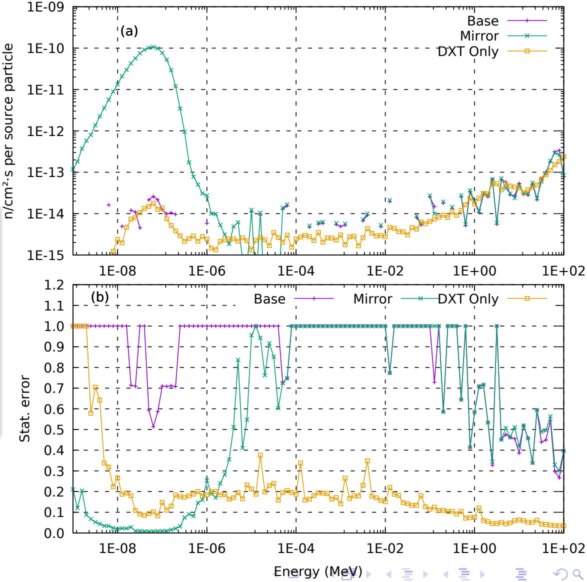

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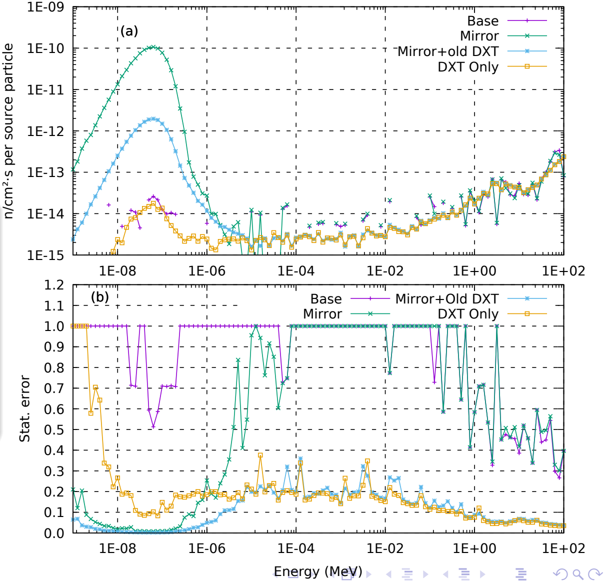

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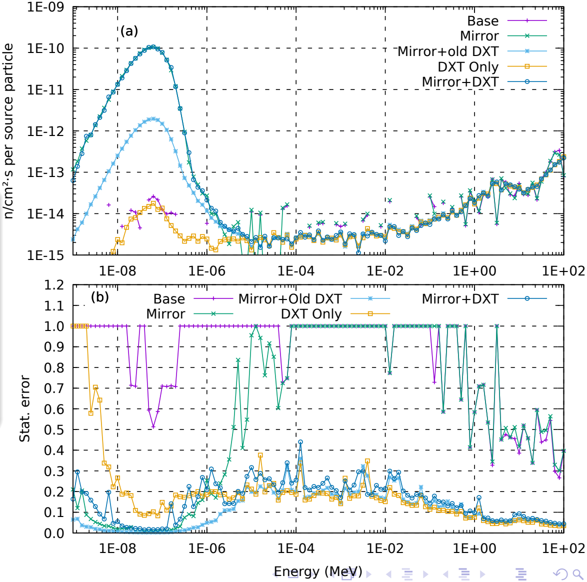
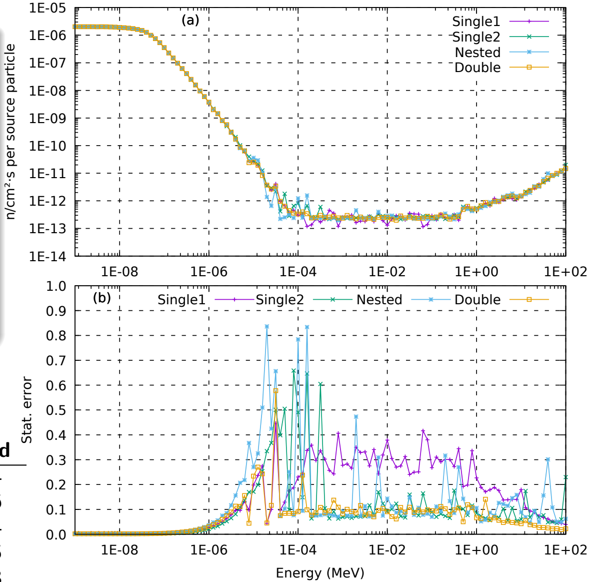


DXT results(Different configurations)

The second set of results compares the different DXT configurations, with also a nested option in order to check for possible unforeseen effects. All configuration give the same spectrum, with the difference being the statistical errors. This shows that the DXT is not skewing the results.

Case	Weight created	Weight destroyed
Single1	4.10E-04	4.10E-04
Single2	8.80E-06	8.76E-06
Double	4.18E-04	4.19E-04
Nested	1.56E-05	1.62E-05
Old DXT	4.09E-04	1.85E-03



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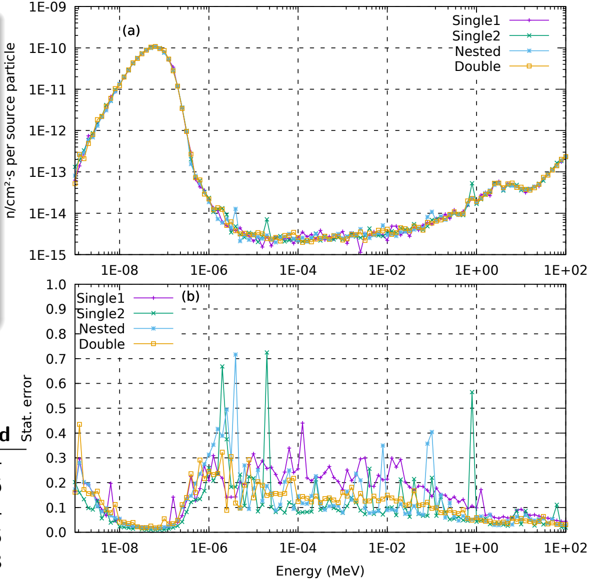
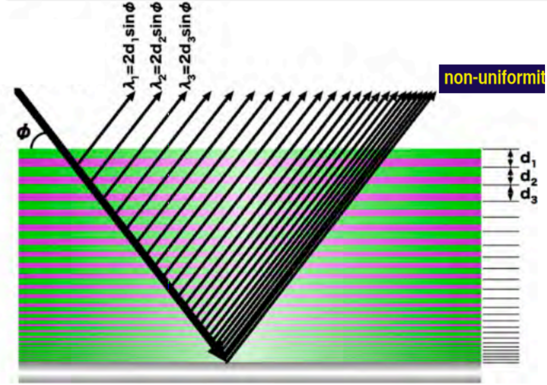


Gamma generation in coatings

Issue and explanation

The Supermirror implementation of MCNP6 (and PHITS) assumes that reflection takes place on the outer surface of the mirror. However, in reality, this is only reasonably true for neutrons below the critical transfer momentum for the material of the outer layer (Typically Nickel) Q_c. Neutrons above that energy penetrate in the Ni/Ti layers of the supermirrors, and are reflected at a depth where the bilayer depth satisfies Bragg's condition.



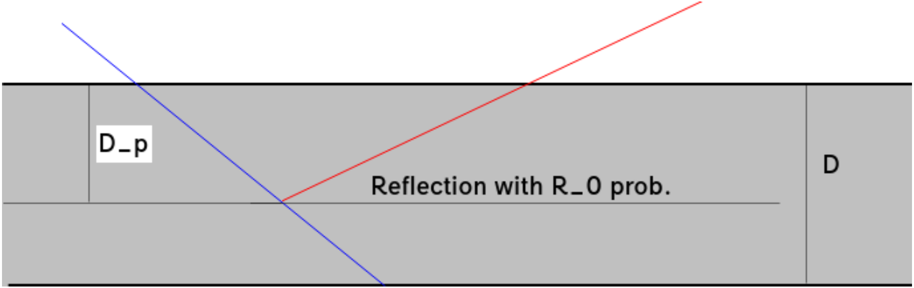
Effects on gamma generation

MCNP6 uses an empirical equation also used by McStas, which is an approximation to the actual reflectivity of the supermirror. Even if this equation is a reasonable aproximation, and the reflection of the neutrons is correctly calculated, the abpsortion of neutrons inside the coating is heavily understimated.

In MCNP, the abpsortion is, aproximately:

In a more realistic representation, however, the abpsortion has two parts, one caused by the transmitted wave, and one caused by the reflected wave.

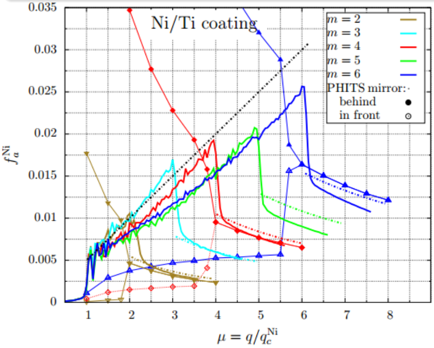
With



Previously proposed solutions

Mirror displacement

It is possible to move the mirror surface to the back of the coating (i.e: Interface between the coating and the substrate), but doing so heavily overstimates the gamma generation, specially for lower Q/Qc values.



From R. Kolevatov
NIMA Volume 922, 1 April 2019, Pages 98-107

Our proposal

A more realistic approach to neutron reflection

In order to have a more realistic representation of reflected neutrons, the idea is having the neutrons make a walk inside the coating that (more or less) corresponds to the actual depth of reflection. Notice that, during that walk, it is possible for the neutron to be scattered, which will cause it to be transmitted since the reflection angles are so low. This effectively reduces reflectivity compared to the equation used.

A Implementation in the software

When a neutron has crossed a surface flagged as a mirror, a property of the particle is activated, which causes an additional track length (DRS) to be defined. This length is a fraction (dependant on Q/Q_c) of the distance to next surface. Because coatings are so thin, the next surface can be assumed to be the coating/substrate interface with a minimal fraction of errors. The walk proceeds as normal, and if DRS is the track length, the reflection subroutine is run. In any case, the flag is cleared for the next track length.

Penetration depth estimation

A critical parameter in this proposal is the fraction of the supermirror depth that the neutron will travel. Because MCNP has no way of simulating the physics at all, an analytical expression must be used. From the Hayter and Mook algorithm, it follows that said depth varies with $(Q/Q_c)^3$. Different algorithms such as Masalovich will have a different penetration depth. However, we believe our calculation will still be a reasonable approach.

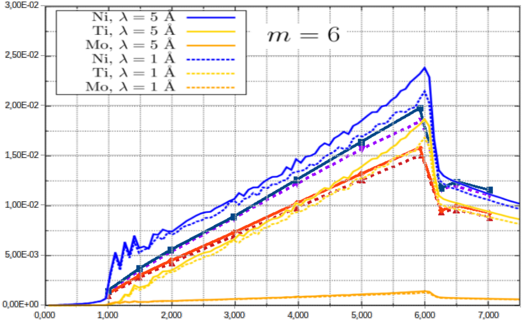
Change in reflectivity

Because we are now transporting the neutron inside the coating, there is an additional loss that reduces reflectivity compared to the McStas formula. Thus, the coefficients of the formula must be modified in order to compensate for this. A spreadsheet to help match provider data has been developed. The reflectivity is no longer Wavelength independent as it used to be the case. While this diverges from McStas, it is ultimately an improvement in the realism of the calculations.

Comparison between QM calculations and MCNP approximation

Graphical comparison

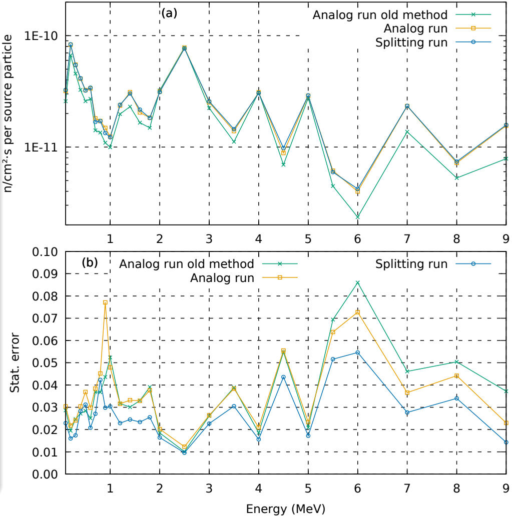
The results are fairly similar in the middle u range. At lower u range, the outer layer of Ni causes a significant difference. At u close to m, the reflectivity of the mirrors does not quite match, with the MCNP adjustment being somewhat lower, causing in turn slightly lower abpsortion. Coating thickness is 12 um.



Gamma generation in the testbench

RFLAG and method effects

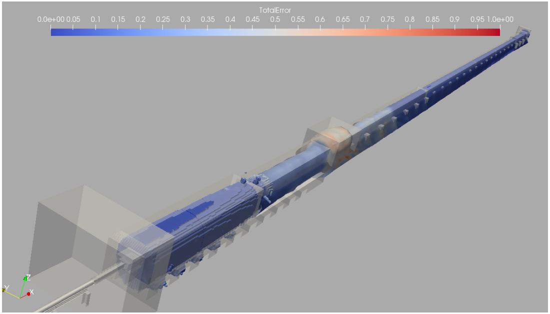
This modification in the logic of the neutron reflection has a visible effect when we look at the gamma generation in the test bench specified before. The difference is specially noticeable at the higher gamma energies (over 5 MeV), which makes sense considering the emitted spectrum from Ti(n,γ) and Ni(n,γ) reactions. While the number of those gammas are few compared to those from absorption in the substrate, their higher energy more than make up for it in terms of dose relevance. Also, notice that RFLAG=2 does improve the statistic for a similar runtime.



Real World usage:MIRACLES

Using the code in a complex scenario

This work has been used for the sizing of the MIRACLES beamline shielding of ESS, starting with source term obtained from the Target Station Model. This is a 150 meter long guide and, as it loses LoS outside the bunker, combines the problematics of high energy neutrons (at the exit of the bunker), neutron scattering (at the chopper pit), and neutron reflection and gamma absorption (through all guide, but specially at the focusing guide). Other variance reduction techniques, such as MAGIC GVR and source splitting are used.



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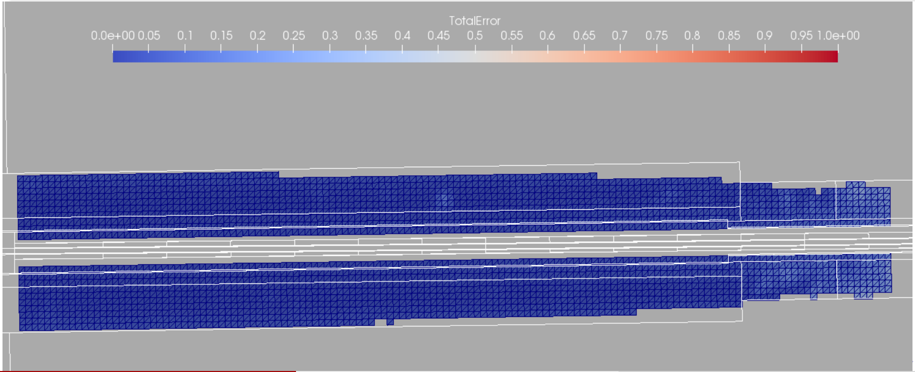

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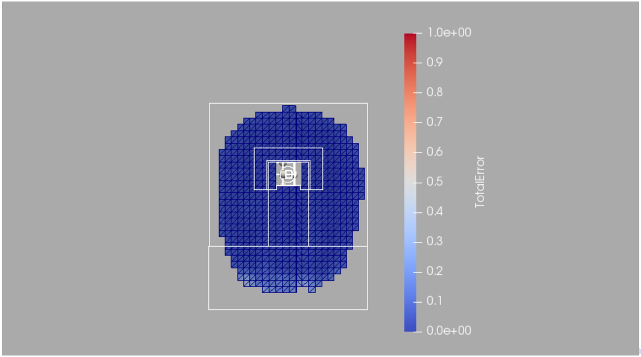

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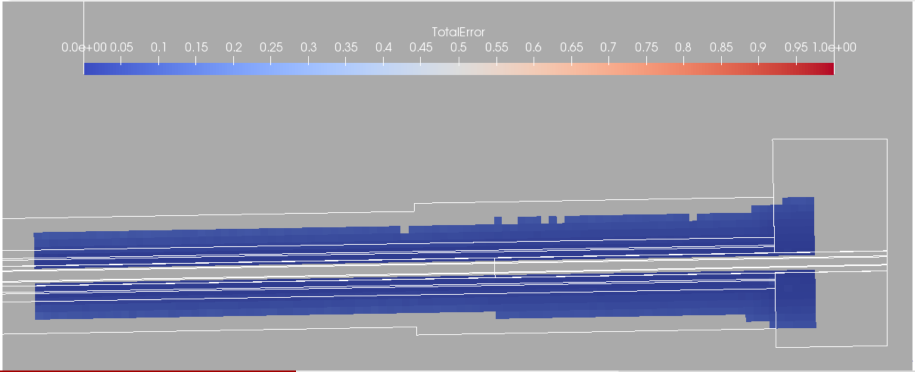

TODO list

Usability Enhancements pendant

- Implement reflection in event log
- Better documentation. Some information exists from previous work, and mostly applies, but we still need to document the new options.
- RFLAG=1 proper testing. This could, for instance, be used to check the abpsortion in the focusing guide very quickly.
- Problem summary accounting. Right now, RFLAG=2 makes the track creation/destruction to differ. This is because the splitting at the mirror has no category to be added to.
- More gracious imcn failure and output information. Getting some of the reflection card wrong ususally results in a segfault. Besides, it is way too easy right now to make mistakes in the reflection surfaces/cells description.

Future work

- Put it to work in a model to estimate instrument noise coming from guide
- Combination with Kyle's chopper work?

ACKNOWLEDGMENTS

SINE 2020

OAK RIDGE National Laboratory

Personal thanks

Fruitful discussions with R. Kolevatov, E. Klinkby and E. Knudsen have been fundamental for this work. The ESS Instrument Common Shielding project staff has also provided useful feedback and information.