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Abstract

The initial thinking behind the deliverable title of "Computational tests, multiple platforms" was to ensure basic platform portability of the developed McStas-MCNP interchange software (MCPL), see Deliverable report D8.2. Given the development synergies achieved with the BRIGHTNESS project and the extent of knowhow brought to table by the WP partners, it became clear that the scope of work could be lifted to a higher level.

After discussions in the WP and detailed discussions between ESS-Bilbao, DTU and the ESS we have therefore adjusted the scope of D8.3 to cover exciting new work on combined support for supermirrors and standard variance reduction techniques within the MCNP6 code:

The design and construction of neutron guides for instruments require biological shielding to protect the personnel from the radiation inside said guides, both coming from the Target station, and generated due to nuclear interactions in the materials of the guide. Calculating it in the design phase is a difficult task, as the problem combines physics from traditional particle transport with neutron mirror physics that are usually featured in specialized codes, and not general transport codes.

In this work we have tested the supermirror patch in MCNP6[1], compared it to previous implementations and introduced some enhancements to improve the statistics in this computationally difficult problem. The resulting tool is then applied with some Variance Reduction techniques to an example of a long guide problem, using the MIRACLES geometry. The results are a breakthrough in shielding analysis for long guides, as integrated, one step shielding calculation is now feasible even for very long guides.

[1] MCNP6: T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L.J. Cox, J. Durkee, J. Elson, M. Fensin, R.A. Forster, J. Hendricks, H.G. Hughes, R. Johns, B. Kiedrowski, R. Martz, S. Mashnik, G. McKinney, D. Pelowitz, R. Prael, J. Sweezy, L. Waters, T. Wilcox, and T. Zukaitis, "Initial MCNP 6 Release Overview", LA-UR-11-07082, Los Alamos National Laboratory, also Nuclear Technology, 180, pg 298-315 (Dec 2012).

Introduction

The development of backscattering instruments, and, in fact, any kind of Time of Flight instrument in general requires the design of a long instrument guide that allows separation of neutrons according to their speed. The inner surfaces of this guide are covered with an extremely polished coat of materials such as nickel/titanium alloy that have the particularity of reflecting low energy neutrons, thus allowing their transport even without direct line of sight. These guides feature a curved design to eliminate the high energy neutrons that are present along with the cold ones in the source.

Because these guides are actually open holes to a high radiation environment, they must be properly shielded to prevent damage to personnel. Design of this shielding using particle transport codes is particularly tricky due to several factors: First, the distances involved are in the order of tens of meters, or even over one hundred. Second, the guide is effectively a very long streaming path that does not quite follow the rules for typical doglegs in nuclear reactors such as those covered in classical guidelines[2]. And finally, the neutron supermirrors physics are not implemented in many of the reference codes for neutron transport. Therefore, very conservative approaches are often taken, as otherwise, it is possible to discover that the radiological dose exceeds the limit during the start-up and additional shielding must be installed.

Aims and Scope

This deliverable first discusses the implementation of a proposed tool to solve this problem, in particular neutron supermirror implementation in MCNPX. It then tests the evolution of this solution, integrated it into a more modern and powerful code base (MCNP6), and presents the improvements that have been implemented in it. It then puts the resulting code in use to calculate neutron transport through the current MIRACLES geometry, presenting the conclusions. The overall scope is thus not just testing existing tools, but to expand and improve them.

Initially existing solutions

F. Gallmeier et al initially worked in a supermirror implementation for MCNPX 2.5 [3], which was later ported to MCNPX 2.7, and tested in the EIGER instrument at SINQ[4], proving that it could accurately simulate neutron mirror behaviour. The implementation reproduces the same equations used by MCStas, allowing easy porting of the conditions to one code from another. However, application of this code to shielding problem requires additional work, as the processes inside the shielding material (nuclear collisions, gamma ray production, etc) must be calculated alongside neutron reflection. Furthermore, the calculations are made more complex as the guide gets longer, and the

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[2] Rockwell, Theodore. Reactor shielding design manual / ed. by T.Rockwell Macmillan London 1956

[3] F. X. Gallmeier, M. Wohlmuther, U. Filges, D. Kiselev & G. Muhrer (2009) Implementation of Neutron Mirror Modeling Capability into MCNPX and Its Demonstration in First Applications, Nuclear Technology, 168:3, 768-772, DOI: 10.13182/NT09-A9304

[4] Bergmann, Ryan & Filges, Uwe & Forss, S & Rantsiou, Emmanouela & Reggiani, Davide & Reiss, T & Stuhr, U & Talanov, Vadim & Wohlmuther, Michael. (2015). VERIFICATION OF THE NEUTRON MIRROR CAPABILITIES IN MCNPX VIA GOLD FOIL MEASUREMENTS AT THE EIGER INSTRUMENT BEAMLINE AT THE SWISS SPALLATION NEUTRON SOURCE (SINQ).

EIGER guide is around 3.6m long, compared to guides over 100m for ESS instruments. Therefore, testing the code in a more representative environment was needed.

For this intention, a simplified geometry representing part of the MIRACLES guide was created. This guide was 76 meters long and featured a curved design to lose Line of Sight. The conclusions from our use were:

- The supermirror physics provide results that are comparable with those of MCSTAS. This is merely a confirmation of previous works.
- MCNPX lacked important features compared to the more modern MCNP6. Among those are the ability to balance the load among processes and the FMESH Mesh tally type.
- DXTRAN Spheres[5] were not compatible with neutron mirror physics for the same reasons that they are not compatible with MCNP implemented ideal mirrors (see MCNP Theory Guide). Because of the geometry of a neutron guide, this technique is extremely useful in solving this problem.

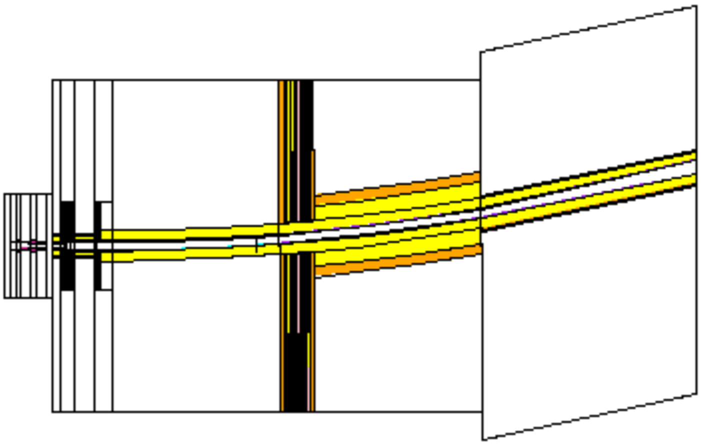

Figure 1: Neutron Guide model used to test MCNPX. Horizontal axis is compressed by a factor of 10.

While some approximations could be made to tackle the problem, the consensus between groups was that improving the existing tools was the more promising option.

Tool port to MCNP6: Testing and results

Recently, R. Bergmann (PSI) ported the supermirror implementation to MCNP6. In order to test this new development, we set a comparison against the existing MCNPX implementation. For this, we

[5] Dxtran is a deterministic transport method typically used for increasing the sampling in a spherical region that would otherwise not be adequately sampled because the probability of scattering toward the region is often very small. Essentially, the dxtran method splits the particle into two pieces at each source or collision point: a piece that arrives (without further collisions) at the dxtran sphere and a piece that does not.
From: Monte Carlo Variance Reduction Using Nested Dxtran Spheres. Available from: https://www.researchgate.net/publication/283167788_Monte_Carlo_Variance_Reduction_Using_Nested_Dxtran_Spheres

run the previous geometry with MCNP6, and compared the results to those of MCNPX at several sections of the neutron guides. The results are summarized in Table

Table 1: Comparison of results of MCNPX and MCNP6 implementation in a full model

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%

Table 2: Comparison of results of MCNPX and MCNP6 implementation in a void model

Tally	Distance (m)	MCNPX Result	MCNP6 Result	% Diff
12	0.5	6.4785E-01	6.4785E-01	0.000%
22	1.5	5.8643E-01	5.8643E-01	0.000%
32	2	9.0645E-02	9.0667E-02	0.024%
42	3	5.2401E-01	5.2394E-01	0.013%
52	7.5	5.0111E-01	5.0106E-01	0.010%
62	9.5	5.0082E-01	5.0077E-01	0.010%
72	25	4.0113E-01	4.0112E-01	0.002%
82	45	2.6035E-01	2.6038E-01	0.012%
92	66	1.7183E-01	1.7185E-01	0.012%

Given the fact that there are some differences in the physics model between MCNPX and MCNP6, the discrepancy seems reasonable. In order to take away that uncertainty, we decided to eliminate all materials in the model and try the result. While such a model lacks any physical meaning, it is a sandbox where we can test the working of neutron mirrors alone. The results reflected on Table 2 are clear: The implementation of Supermirrors in MCNP6 reproduces exactly the MCNPX implementation behaviour.

Improvements to the tool: Deterministic transport

An improvement upon the existing code is to add the option of a deterministic neutron transport through the guide: the traditional, stochastic transport involves the call to a random number generator to check whether a particle will be transmitted or reflected when arriving at a mirror surface, with the reflection ratio depending on the mirror characteristics and the particle momentum. The deterministic method, on the other hand, reflects the particle and then reduces its weight (as defined in Monte Carlo method) by the reflecting ratio. The transmitted particle carrying the rest of the weight can optionally be transported, depending on user needs. This method is deterministic because, once a particle is given a position and speed, no random numbers are used.

However, a small exception must be added in order to the code to work: Particles can not be allowed to reduce their weight by so much that the resulting floating-point representation equals to zero, as this causes an immediate crash in the code. Therefore, an exception is added with particles with extremely low weight, to use stochastic transport. Because those particles are insignificant compared to the average weight, the result is, in practice, deterministic.

The advantages of these approach mimic those of the deterministic approach of DXTRAN: high weight particles with a very low chance of being produced are replaced by a large amount of small weight particles that are generated at each event, with the aforementioned roulette for low weight particles being the equivalent of the detector roulette. Figure 2 illustrates the improvement obtained in a guide simulation from using this approach Vs. classical stochastic approach. Notice, however, that while there is a significant advantage, this approach by itself is nowhere near of giving a full solution to the problem.

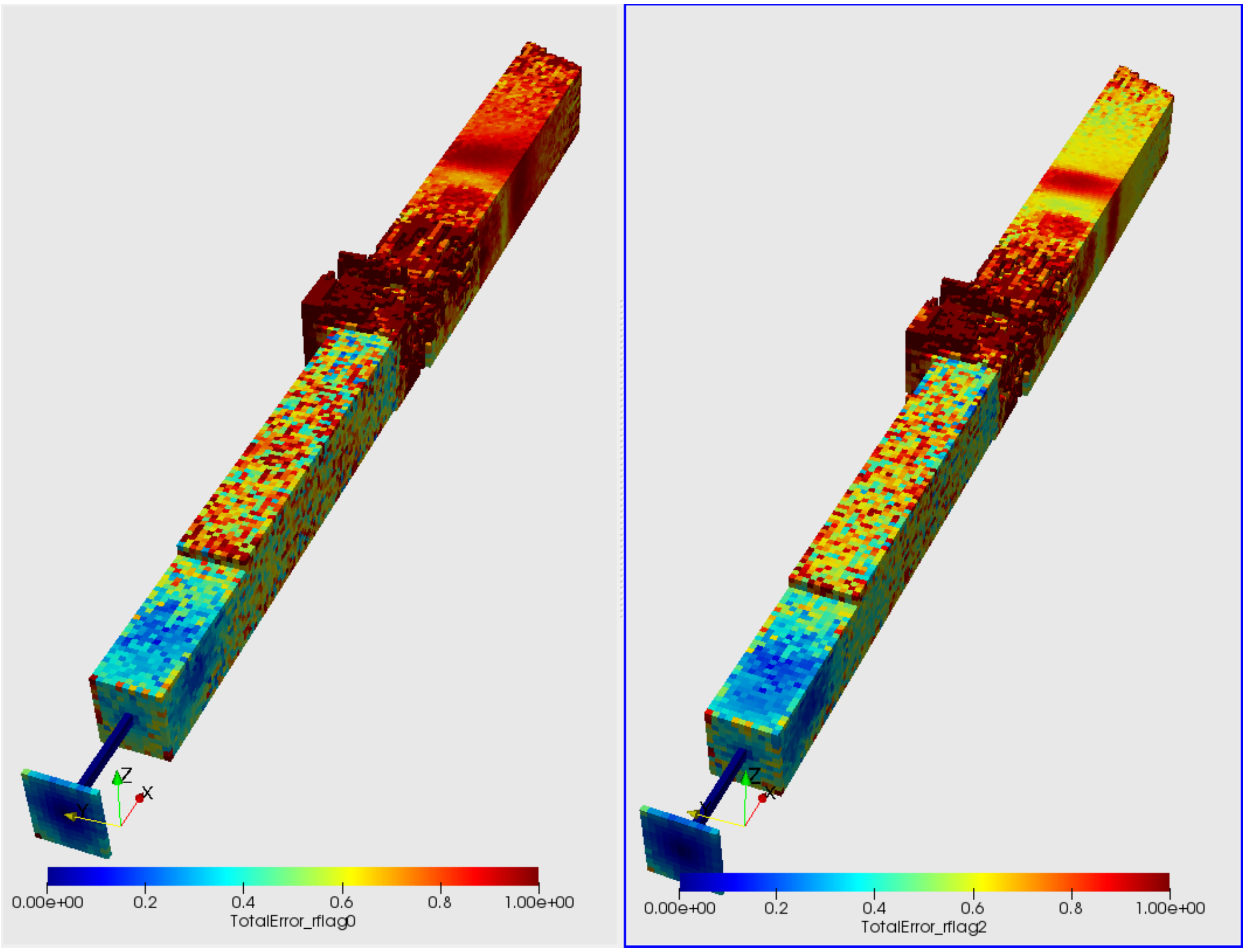

Figure 2: Comparison of stochastic (left) Vs deterministic guide reflection. Relative errors.

The next improvement was to make DXTRAN spheres compatible with neutron reflection. For this purpose, further modification of the code was made as following:

- An additional property of the particle (reflected) was defined. This property is an integer set to 1 for particles that just underwent a reflection, and to 0 otherwise.
- Source particles are always born with reflected=0
- Whenever a particle crosses a mirror, the reflected particle (if it exists) is set to reflected=1
- Whenever a particle undergoes a collision, it is set to reflected=0. Notice that this is inherited by any particle resulting from an (n,xn) reaction.
- Particles with reflected=1 do not “see” DXTRAN spheres. Notice that the codebase for this is actually present in MCNP6.
- A particle that has gotten inside a DXTRAN sphere (via mirrors) will not interact with it, but will still contribute to other spheres.

As a result, the DXTRAN effectively stops existing for reflected neutrons but is still present for the rest. Notice that, if using the deterministic reflection approach implemented, DXTRAN becomes redundant for those neutrons.

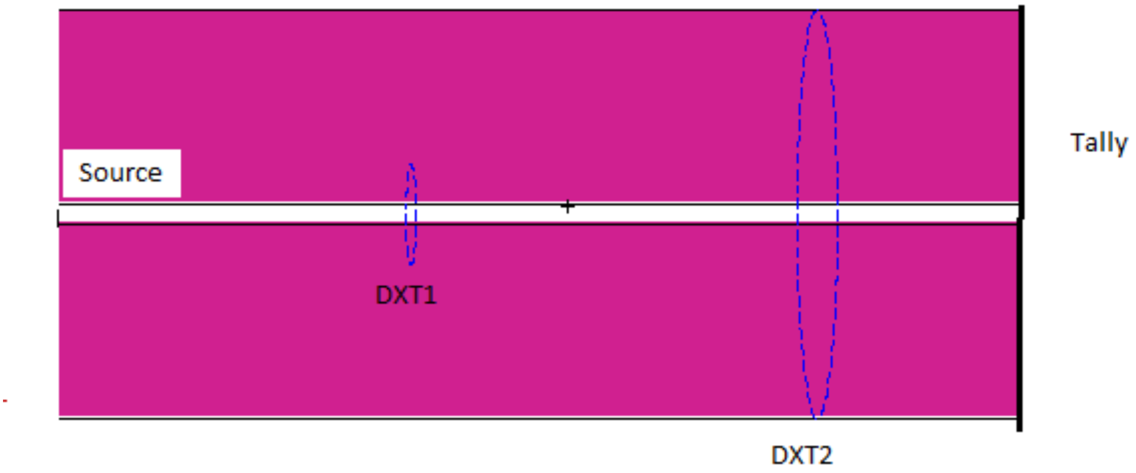

Figure 3: DXT test model. Notice that horizontal axis has been compressed by a factor of 10.

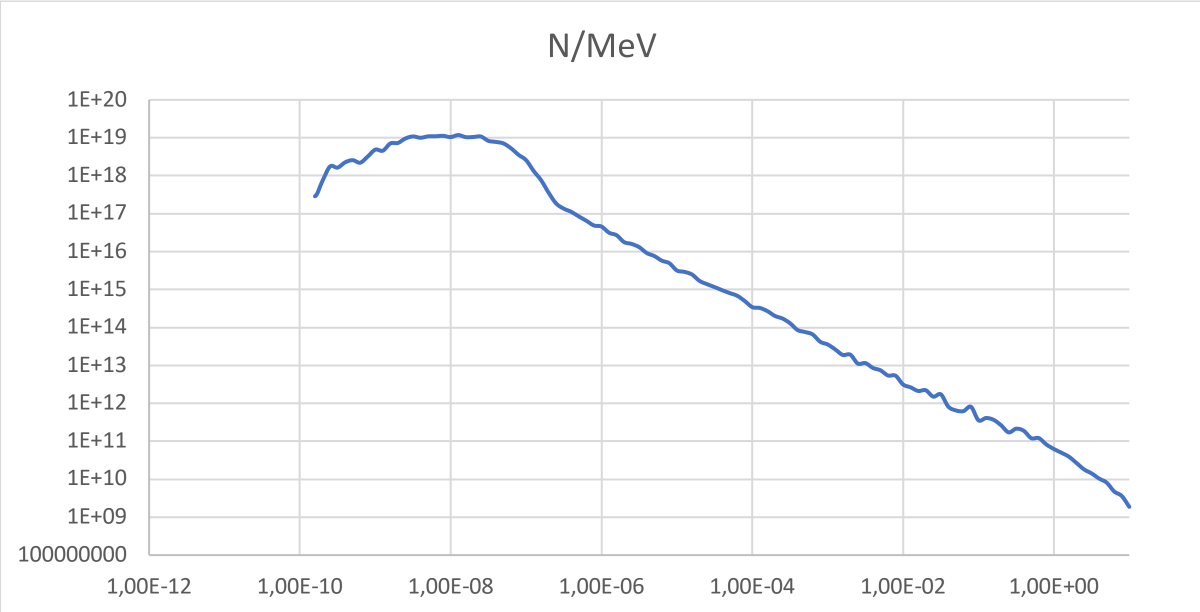

Figure 4: Neutron spectrum for the DXTRAN test (energy in MeV)

The code has been tested in a simple, easily trackable problem featuring 2 spheres, depicted in Figure 3. The problem has a point source with a uniform angular distribution in a 1-degree cone coaxial through an m=2 cylindrical, 1cm radius guide. Source energy distribution is represented in Figure 4. The material surrounding the guide is either carbon steel or void, depending on setup. The void setup is obviously non-physical, but allows us to test the working of the code. The results of the flux at the back end of the geometry have been compared, as well as the weight created and destroyed by DXTRAN.

Results are reflected in Table 3

Table 3: DXTRAN spheres test results.

	Simulation with material	Void simulation
Flux at the back	4.95E-8	8.06E-4 n/sp
Flux at the back W/O DXTRAN	4.93E-8	7.50E-4 n/sp
DXTRAN weight generated	2.78E-2	1.51 /sp
DXTRAN weight destroyed	2.79E-2	1.44 /sp

The results show that, in the void scenario, the DXTRAN creates a significant amount of weight. The reason for that is an excessive contribution in a particular scenario: When the contribution track crosses a mirror from the guide, its weight is not reduced by the corresponding reflectivity, while the actual chance of arriving to the sphere is.

In a physical setup, the importance of this is minimal to non-existent: The working angle of the mirrors is very small, creating a tight geometrical constraint. On top of that, neutron energy needs to be low, which means that the cross-sections, and thus the attenuation to the sphere, will be high,. The void simulation obviously has no such constraint, and thus it makes the discrepancy artificially high.

Notice that the code has NOT been tested for nested DXTRAN spheres, so the authors can not guarantee its correct working if using this feature.

Application to a real-world scenario: The MIRACLES instrument

With the above developments, the code has been put to use in a real geometry. In particular, a model representing the full guide of MIRACLES was created using SuperMC[6] from the design CAD using some simplifications. The model features over 150m of guide, using supermirrors of different characteristics. Steel and concrete are used for shielding, using a preliminary, experience-based design. The bunker wall is modelled as a solid 5m wall, but gaps are featured around the guide. As the source term for MIRACLES is still under calculation, the source for NMX, calculated by D. DiJulio is used. The model is enclosed in a 6 meter wide box, and all radiation beyond that is considered lost, as is any neutron whose energy falls behind 0.1 meV. ENDF-B/VII libraries have been used for the calculations. The DMSC cluster has been used for the calculations.

Several Variance Reduction methods are combined:

[6] "Y. Wu, FDS Team, CAD-based interface programs for fusion neutron transport simulation, Fusion Engineering and Design 84 (2009) 1987 – 1992

- A MAGIC[7] Weight Window generation is used. This method has been used by the ESS-Bilbao team in several calculations performed for the ESS Project and offers a global improvement throughout the entire geometry.

- This weight window has been further tuned using and exponentially attenuated upper cap, which limits the maximum value of the weight window to a value which decreases exponentially as the weight window advances through the guide.

- The higher energy (over 10 MeV) part of the source has been separated and put into a different simulation. This is because these high energy neutrons have a) very low sampling in the total source b) High penetrating power that makes them behave in a quantitatively different way.

- Computing-time saving measures such as exponential transform in the bunker wall and roulettes have been used to keep the histories from getting too long.

The geometry of the file is represented in Figure 5. The X axis has been compressed by a factor of 10 for convenience.

[7] A. Davis and A. Turner. Comparison of Global Variance Reduction methods for Monte Carlo Radiation Transport Simulations of ITER. In Proceedings of the 26th Symposium on Fusion Technology - SOFT-26, 2010

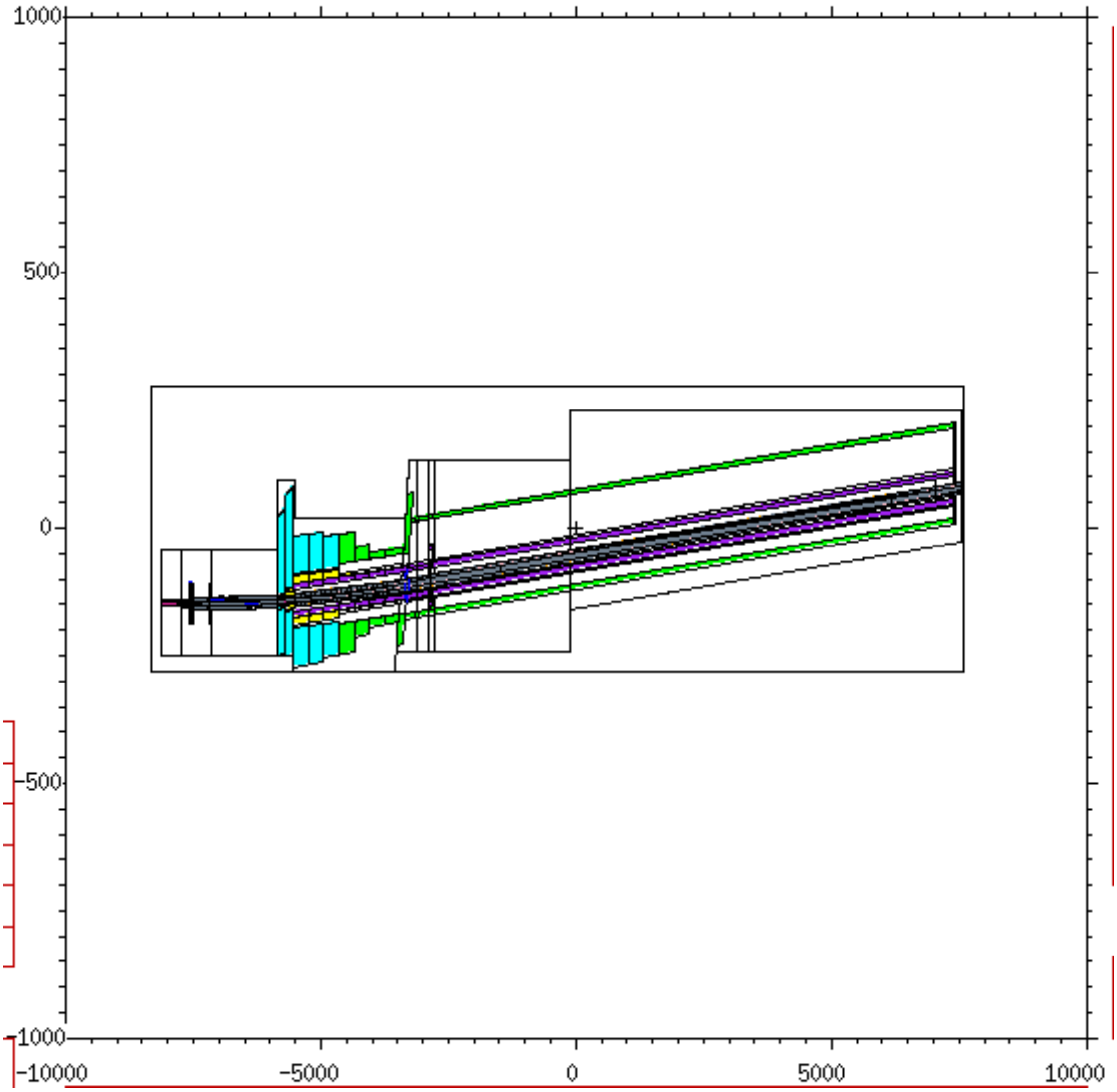

Figure 5: Full current MCNP model for MIRACLES

Notice that even the combination of these methods, without the added value of the deterministic transport developed in this work, did not suffice to get meaningful results through the entire guide. It is the combination of all these techniques that have allowed us to achieve the solution.

Figures show different parts of the neutron flux map. Because of the size of the problem, it is virtually impossible to explain every single detail in this document. However, the most important remarks we need to make are:

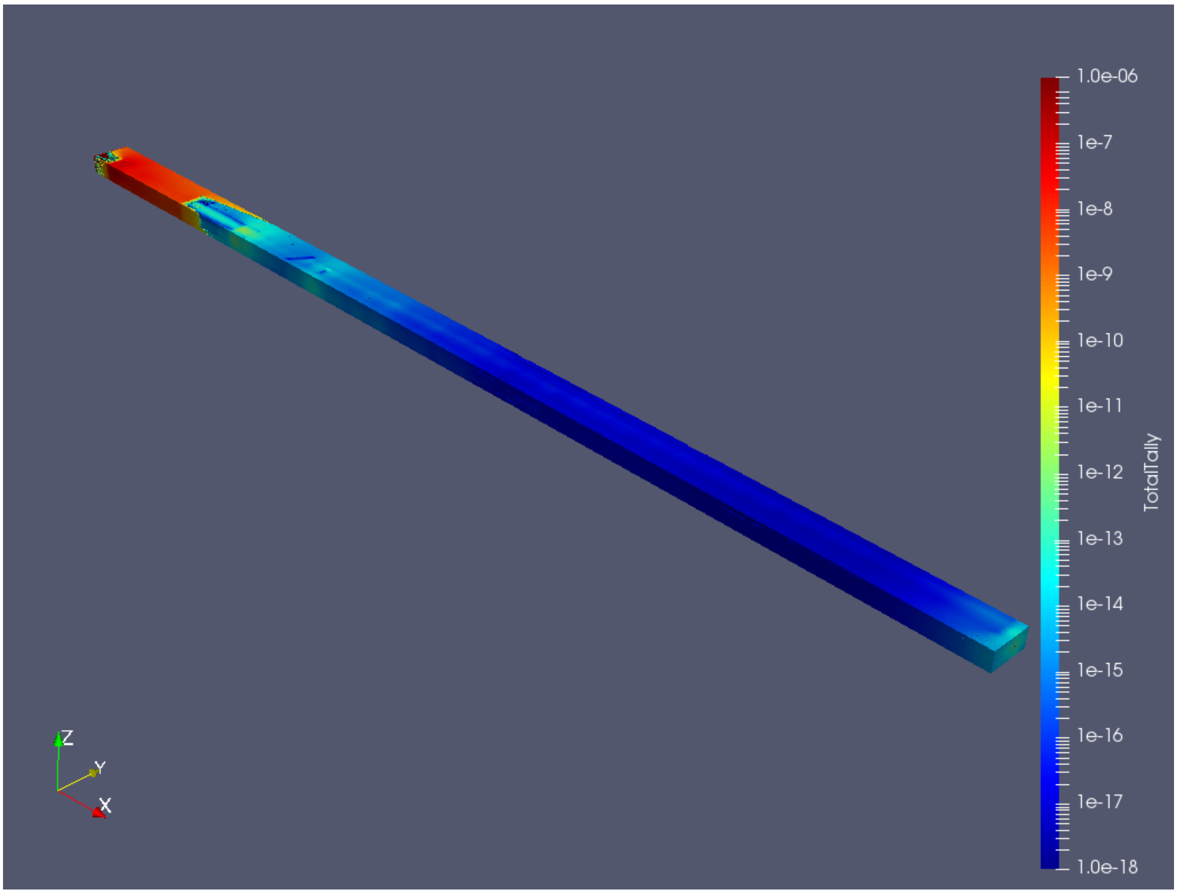

Figure 6: Neutron flux (per source particle) through the MIRACLES geometry, general overview.

1. The code gets results, with uncertainty in most volumes below 0.1, throughout the 150m of the guides, in a 10x10x10cm cartesian mesh.

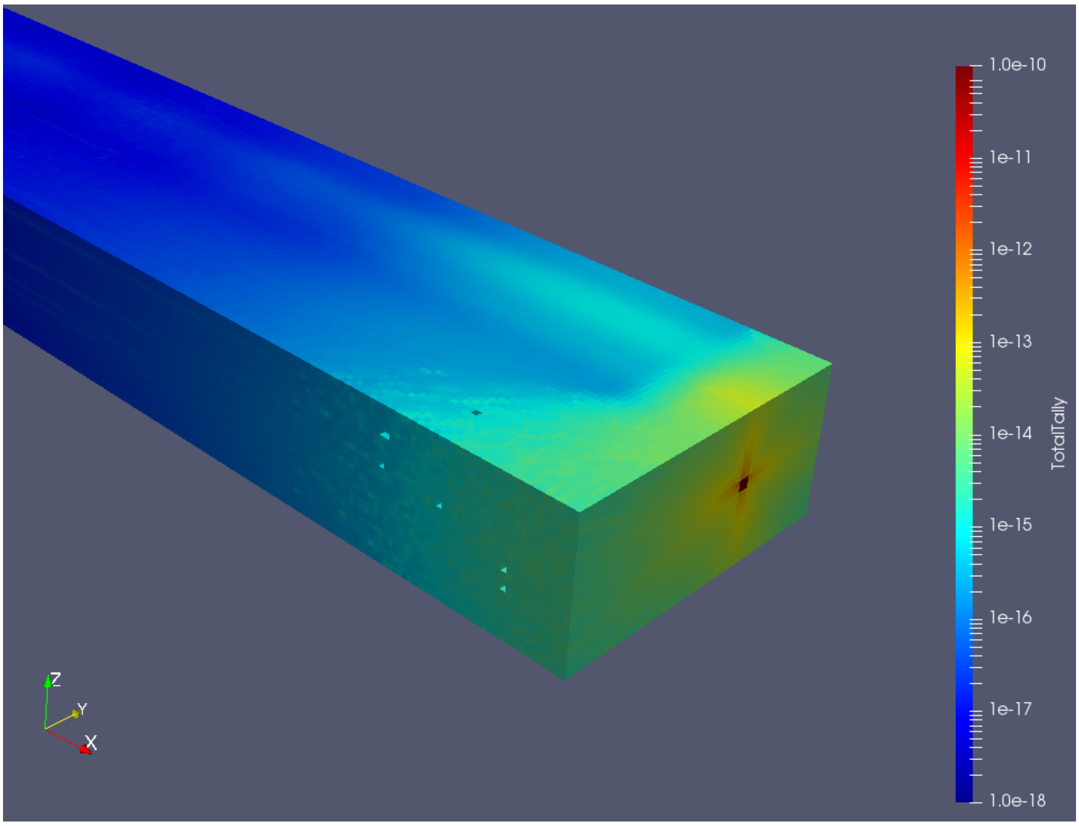

Figure 7: Neutron flux (per source particle) in the MIRACLES Geometry: detail at the end of the guide.

2. The code is able to reflect the expected increase at the end of the guide due to its focusing and the neutron leakage.

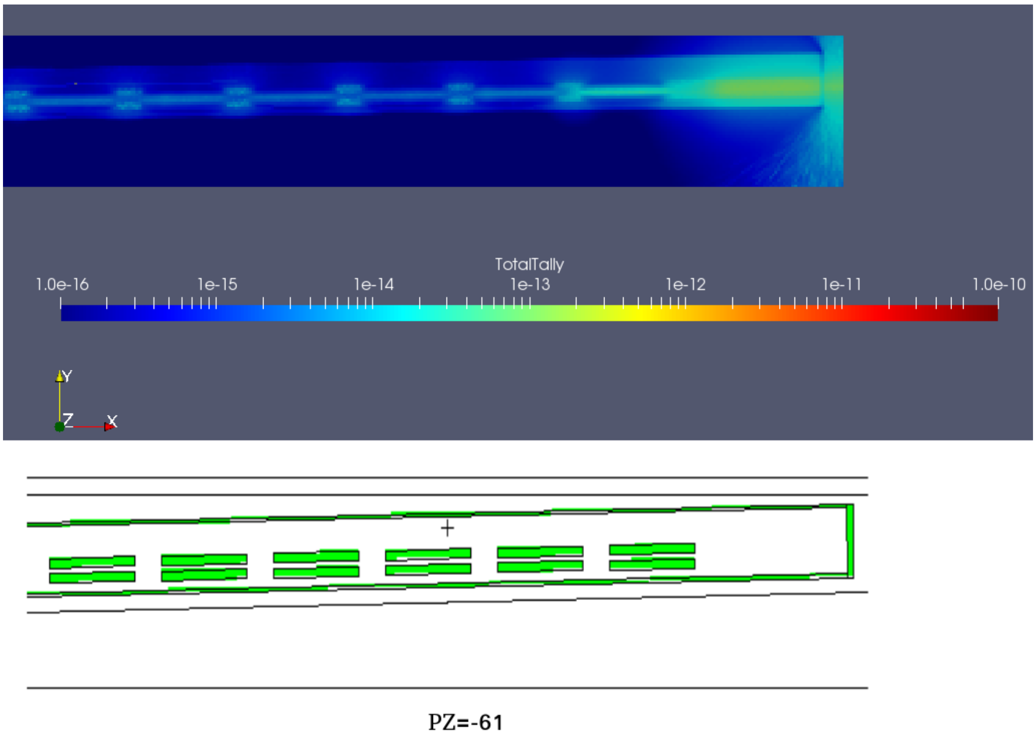

Figure 8: Neutron source (per source particle) in the MIRACLES geometry. Z=-61 slice.

3. Even at the end of the guide, the results of flux make the "shadow" of the designed supports clearly visible, indicating that we are able to get a significant amount of tracks even at that length.

4. Radiation creation at features like neutron choppers is clearly visible and solved. Thus, we will be able to optimize the shielding needed.

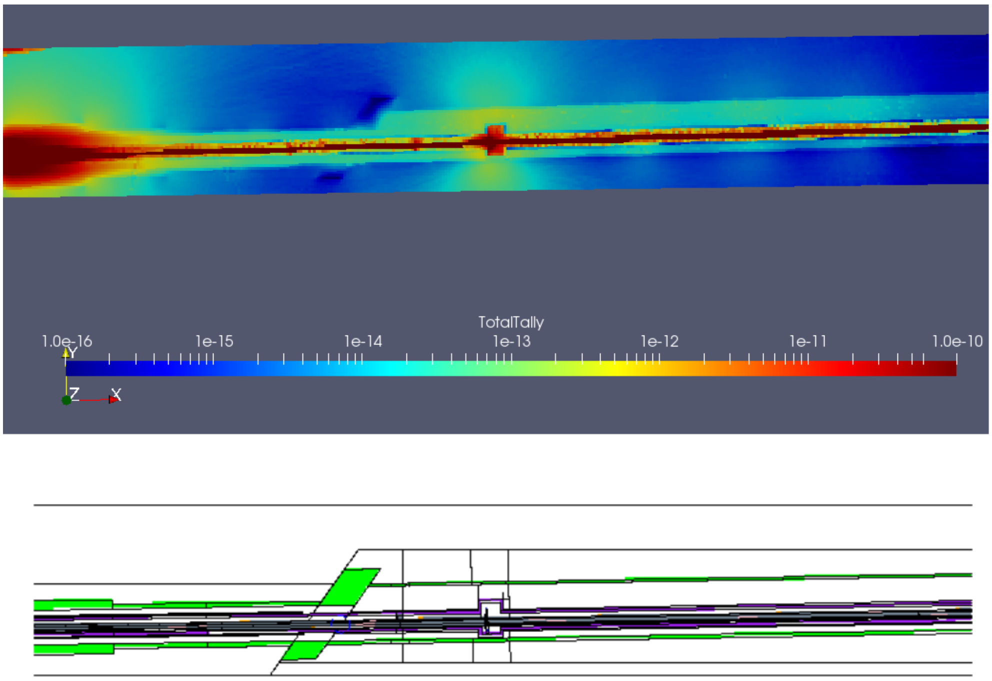

Figure 9: Neutron flux in the MIRACLES geometry: Detail at Chopper #3

5. The combination of weight windows and DXTRAN enables calculations down to a very low flux: The source term multiplier to use in this case is 1.65E13, which means that we are able to resolve neutron fluxes in the order of 1E-2n/s·cm^2, which is more than enough to calculate shielding to the target value of <3 microSv/h

Overall, this shows that the developments in the code enable the users to perform single-stage, integrated calculations of long guides, which is a sizable advantage for shielding design and noise calculation.

Future developments

In order to provide insights of the behaviour of the neutron mirrors, an output table, featuring information about reflection and transmission taking place in each of the surfaces, is planned. This table is intended to help users to understand the events taking place, in a similar way other MCNP tables do.

The ESS-Bilbao team is working at the time of writing this document in further detailing the MIRACLES model with features such as B4C lining and will perform full transport simulation including generation of gamma rays. As nested DXTRAN spheres have been proved to be useful in streaming problems with extremely long paths[8], we intend to test them and explore the possibility of using them.

. The authors look forward to making the code available to other teams in similar works, within the MCNP license Framework and with permissions from the other contributors.

Finally, the authors look forward to benchmark and compare this code with the proposals of other teams for similar problems.

Conclusions

- Existing MCNPX patch was tested, and its potential improvements were identified.
- A new version of the patch for MCNP6 was tested and its results compared and validated with previous version.
- Improvements on this code were made that significantly increases its power.
- The combination of these improvements with other VR techniques enables us to perform single-stage, integrated shielding analysis in long guides. This allows us to optimize shielding in areas where we pretty much had to ballpark or trial/error before.
- This development can benefit all the teams that need to design a long guide, so the contribution benefits the entire ESS project in particular, and the know-how of the community in general.

Acknowledgements

The authors want to thank Dr. Ryan Bergmann (PSI) for his work in coding the core mirror physics in MCNP6, and the fruitful discussions held, and Dr. Esben Klinkby for his help in communication, as well as the DMSC division of ESS for making the computing resources available.

[8] T. E. Booth, K. C. Kelley & S. S. McCready (2009) Monte Carlo Variance Reduction Using Nested Dxtran Spheres, Nuclear Technology, 168:3, 765-767, DOI: 10.13182/NT09-A9303