Benchmarking Geant4 for spallation neutron source calculations

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Abstract. Geant4 is becoming increasingly used for radiation transport simulations of spallation neutron sources and related components. Historically, the code has seen little usage in this field and it is of general interest to investigate the suitability of Geant4 for such applications. For this purpose, we carried out Geant4 calculations based on simple spallation source geometries and also with the European Spallation Source Technical Design Report target and moderator configuration. The results are compared to calculations performed with the Monte Carlo N-Particle extended code. The comparisons are carried out over the full spallation neutron source energy spectrum, from sub-eV energies up to thousands of MeV. Our preliminary results reveal that there is generally good agreement between the simulations using both codes. Additionally, we have also implemented a general weight-window generator for Geant4 based applications and present some results of the method applied to the ESS target model.

1. Introduction

Spallation neutron sources are powerful tools for materials research. These sources generate low-energy neutrons for scientific investigations through the bombardment of a heavy metal target with a high-energy proton beam. A popular set of software, used in the design of modern-day spallation sources, is the Monte Carlo N-Particle Transport extended code (MCNPX) \cite{1, 2}. For example, the baseline design of the upcoming European Spallation Source (ESS) \cite{3} and the subsequent optimization of the moderators were performed with MCNPX \cite{4}. The reliance on MCNPX is partly based on it’s history of benchmarking and validation, use of data driven libraries, and implementation of high-energy cascade models. Of specific interest are the pre-packaged libraries for the interactions of low-energy neutrons in materials, which compose the primary signal for materials science investigations. These are critical for calculations of moderator performance.

Geant4 \cite{5, 6}, which is a popular simulation toolkit particularity in the high-energy physics realm, has seen little application in the field of spallation neutron sources. There are however a number of reasons why it is of interest to investigate the suitability of Geant4 for spallation neutron source calculations. For example, in the recent years there has been an influx of new ideas, especially from high-energy physics labs such as CERN \cite{7}, directly into the neutron scattering community. Geant4 is also open source, freely available online, and supported by a large user community spanning a broad range of scientific fields. Lastly, modern day spallation sources
are reaching energy ranges which are commonplace in the high-energy physics community. The Materials and Life Science Experimental Facility [8] at the Japan Proton Accelerator Research Complex (J-PARC) [9] employs a 3 GeV proton beam and the ESS will use a 2 GeV proton beam.

At ESS, there is a significant push towards building on-top of the experiences from the high-energy physics community and developing Geant4 to meet the requirements for neutron instrument detector design [10, 11]. Additionally, Geant4 is employed at ESS for calculations of the neutronic response of the shielding components of neutron scattering instruments [12, 13, 14, 15]. These two points make it possible to simulate in detail the areas where the cross-talk between radiation background levels and neutron detectors is critical for the performance of an instrument. A key question which could be asked is then how well does Geant4 simulate the spallation neutron source environment, compared to the often used MCNPX code?

The aim of the present work is to investigate the suitability of Geant4 for spallation neutron source calculations and benchmark it against MCNPX. Three test problems were selected for comparison of the two codes. The first is a simple spallation target model and the second is the spallation target model combined with a single para-hydrogen moderator. We selected the ESS baseline design highlighted in the Technical Design Report [3] for the third comparison. In the following, we present the general features of the two codes relevant for this work and the results of the three test scenarios. We focus primarily on the production of neutrons which are important for both the signal used for materials science investigations and also the background noise. Lastly, we also present an implementation of a general weight-window generator for Geant4 based applications, in particular to be used for deep-shielding calculations.

2. Details of the Monte-Carlo software
The MCNPX calculations were performed using version 2.7.0. The default nuclear interaction Bertini model [16, 17] coupled with the ENDF/B-VII.0 [18] neutron libraries was used. At thermal energies and lower, the neutron transport was handled by the prepackaged neutron scattering kernels. These were activated for hydrogen in para-hydrogen and light water, beryllium, aluminum-27, and iron-56 in the iron and steel.

The Geant4 calculations were carried out using Geant4 version 10.0 patch 3. The physics list QGSP_BERT_HP was used for the calculations [19]. This list is one of the recommended lists for shielding applications [20]. QGS stands for the quark-gluon string model, P for precompound, BERT for the Bertini intra-nuclear cascade model, and HP for the high-precision neutron package [19]. The HP package uses evaluated neutron data, named G4NDL4.4, for interactions of neutrons below 20 MeV. This data largely comes from the ENDF/B-VII.0 libraries. Included
3. Simple spallation source models

The first test of the two codes was carried out on a simple tungsten target which was 2 m in diameter. The Geant4 rendered geometry is shown in Fig. 1. The energy of the primary proton beam was 2 GeV. The energies and directions of neutrons leaving the top surface of the target also in this package is data for the thermal scattering of neutrons below 4 eV.

Finally, we mention that the Geant4 simulations were carried out using the ESS Detector Group framework [10]. The framework provides a Geant4-based Python/C++ simulation environment which offers a number of developments to aid neutron detection and shielding calculations. The results presented here were carried out within this framework, however no additional features were implemented beyond what is contained within the standard Geant4 release.
Figure 3: Rendering of the simple spallation source target model and moderator used in the Geant4 calculations.

were saved for the comparison and the results are shown in Fig. 2. The four spectra in the figure show the energies of neutrons leaving the top surface of the target and their directions. The z-direction is along the proton beam axis, the y-direction is along the height of the target, and the x-direction along the width of the target. Overall there is excellent agreement between the results of the simulations using the two codes.

The second test model was the simple tungsten target combined with a liquid para-hydrogen moderator and is shown in Fig. 3. Information regarding the neutrons leaving the side surface of the moderator was saved for comparison of the results of the two codes. Generally, there is again good agreement between the results of the two codes. One can note in particular the excellent reproduction of the moderator peak in the low-energy spectrum, which is of particular interest for neutron scattering studies. The neutron directions are also reproduced well by Geant4.

4. ESS TDR model

The third model tested in this work was the ESS TDR design of the target and moderators, described in Ref. [3]. The neutronic design of the model was carried out using MCNPX as the primary simulation code. The MCNPX model of the target zone is shown in Fig. 5. The proton beam from the accelerator, parabolic in shape with a width of 16 cm and a height of 6 cm, impinges on an 8 cm tall helium-cooled rotating tungsten target. The diameter of the wheel is 2.5 m. Above and below the target are positioned volumetric moderators of cylindrical shape with a diameter of 16 cm and a height of 13 cm. The moderators contain super-critical para-hydrogen and are partly covered by ambient light water premoderators with wings which have thicknesses of 4 cm. These make it possible to extract both cold and thermal neutrons for a single beamline. Extending from the moderators are four extraction areas of 60° for the neutron beamlines. A beryllium inner reflector, a stainless steel outer reflector, and iron shielding surround the moderator region.

The ESS TDR geometry was also implemented into a Geant4 model and the preliminary results of the Geant4 simulations compared to the MCNPX simulations are shown in Fig. 6. The energy spectra are the sum over all the neutrons leaving the four 60° extraction areas at a distance of 2 m from the moderators. While there is good agreement between the spectra, work is still underway in refining the geometry of the Geant4 model to more closely match the MCNPX model. At this moment in time, there is no tool that the authors are aware of that makes the transition from one geometrical model in MCNPX to Geant4 a simple procedure. The preliminary results presented here are however very encouraging.
5. Automated variance reduction methods

In addition to the benchmarking tests described above, we have also investigated the suitability of Geant4 for weight-window based calculations. While Geant4 supports the usage of the weight-window technique, it however does not come equipped with a weight-window generator. Therefore, we have implemented an automated variance reduction method for Geant4 based applications. These methods are of particular interest for deep shielding calculations, which are required for both safety reasons and estimates of instrument backgrounds due to leakage of high-energy particles from the shielding components. The implemented approach is described in detail in Ref. [15, 21] and will be briefly summarized here. The approach uses a Global Variance Reduction (GVR) method to encourage the uniform population of particles throughout a model geometry and is based on the weight-window technique. The steps for the procedure are

Figure 4: Results of the MCNPX and Geant4 calculations for the simple spallation source target and moderator model shown in Fig. 3. The energy spectrum of the neutrons leaving the target are shown in the top left panel, the x-directions of the neutrons leaving the target in the top right panel, the y-directions in the bottom left panel, and the z-directions in the bottom right panel.
Figure 5: The left panel shows a vertical cut through the axis of the moderators in the MCNPX model and the right panel shows a horizontal cut.

described below:

1. A weight-window and scoring mesh are defined and overlaid across the mass geometry of the model.

2. An analog run (i.e a run with the weight-window technique disabled) is performed and a log file is stored which contains the relative errors and fluxes of each cell in the mesh.

3. The stored log file is then used by the application to calculate the weight-window limits using either of the following equations

$$W_L = \left( \frac{C_U + 1}{2} \right) - 1 \frac{\text{Min}(\vec{R}e)}{\vec{R}e_i}$$

(1)

or

$$W_L = \left( \frac{C_U + 1}{2} \right) - 1 \frac{\phi_i}{\text{Max}(\phi)}$$

(2)

where the first is known as the flux-based method and the second as the relative-error based method [22]. The parameter $W_L$ is the weight-window lower bound, $C_U$ is a parameter defined by the user, and $\vec{R}e$ and $\phi$ are vectors with the relative error or flux information of the defined cells in mesh, respectively. The first method encourages a uniform population of Monte-Carlo particles throughout the geometry while the latter encourages a flat distribution of errors throughout. The user can choose either method in the code. After the weight-window run is carried out, a new log file is written which can be used for more iterations of the procedure.

Figure 7 shows a selection of flux maps and relative error maps for an analog simulation compared to a GVR simulation using the flux-based approach and applied to the Geant4 ESS TDR target and moderator model for simulations of a similar time. The maps represent a plane above the target center. The black circular regions mark the ends of the monolith inner iron and outer concrete shielding. In the given simulation time, the GVR simulations lead to a nearly
6. Conclusions
In the current work, we presented results of simulations of simple spallation targets and the ESS TDR design using the Monte-Carlo codes Geant4 and MCNPX. Overall, there is in general good agreement between the results shown in this work. Additionally, we presented an implementation of an automated weight-window generator for shielding applications and showed the benefit of using the approach compared to analog simulations. The above mentioned developments suggest that Geant4 is well suited for spallation neutron source related calculations.

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Figure 7: Flux and relative errors maps for a plane in the Geant4 ESS TDR model using an analog simulation and a simulation using the GVR approach. Panel a) shows the flux map for the analog simulation, panel b) the relative error map for the analog simulation, panel c) the flux map for the GVR method, and panel d) the relative error map for the GVR method.

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