Validation of the performance of Geant4 in the simulation of neutron induced reactions relevant to reactor studies.

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Abstract. Geant4 is a Monte Carlo simulation toolkit that is used for the simulation of particles through matter. It was developed by a world wide collaboration of about 100 scientists. It has applications in high energy physics, astrophysics, medical physics, nuclear physics experiments, accelerator and space science studies. The Evaluated Nuclear Data File, ENDF/B-VII database is included in the simulation toolkit, making it feasible to use the Geant4 toolkit for low energy neutron-physics simulations. The ENDF/B-VII database stores evaluated nuclear reaction data files from the major evaluated libraries. In this presentation Geant4 was used to perform simple single event neutron scattering simulations on materials that are typical for a nuclear reactor. Some of the materials used are found in the SAFARI 1 reactor at Necsa, Pelindaba. These include Aluminium, Beryllium. This was done in order to validate the Geant4 implementation of primary processes relevant to reactor studies within the ENDF/B-VII database of cross sections.

1. Introduction

Geant4 is a Monte Carlo based simulation toolkit that is used for the Geometry and Tracking of particles through matter. Although initially developed for high energy physics it has been extended and it has capabilities for applications in the low energy physics spectrum [1]. It is an open source modern object oriented code. It has proven success at a very high level of complexity for the geometry construction, materials specification, tracking algorithms and the physics lists in the high energy physics regime [2].

The energy loss of neutrons is mainly due to elastic scattering, absorption and nuclear collisions [3]. A typical nuclear reaction is written as [4]:

$$a + X \rightarrow Y + b \tag{1}$$

where a is the incident particle and X is the target and Y and b are the reaction products. If the outgoing and the incident particles are the same i.e Y and X are the same nucleus then the nuclear reaction is a scattering process. If Y and b are in their ground states it is an elastic scattering.

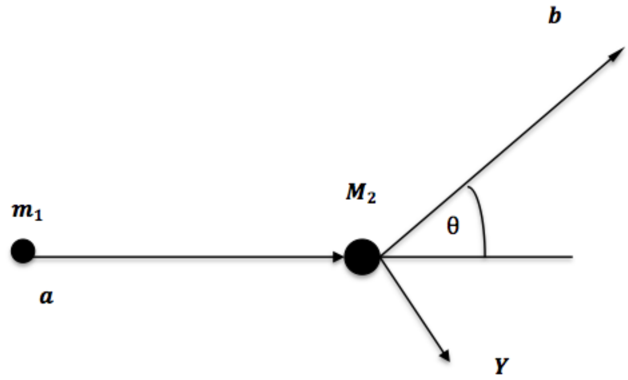

Figure 1. Kinematics of a nuclear reaction of the type a + X → Y + b, where m_1 is the incident particle, M_2 is the target nucleus, θ is the scattering angle, Y and b are the reaction products.

Conservation of total relativistic energy in a basic reaction is:

$$m_X c^2 + E_X + m_a c^2 + E_a = M_Y c^2 + E_Y + m_b c^2 + E_b \tag{2}$$

where the $E^{'}s$ are the kinetic energies and the $m^{'}s$ are the rest masses [4]. The Q value which may be positive, negative or zero becomes:

$$Q = \{m_{initial} - m_{final}\}c^2 \tag{3}$$

This is the same as the access kinetic energy of the final products:

$$Q = E_{final} - E_{initial} = E_Y + E_b - E_X - E_a \tag{4}$$

Conservation of linear momentum (p) along and perpendicular to the beam direction is given by:

$$p_a = p_b cos\theta + p_Y cos\phi \tag{5}$$

and

$$0 = p_b sin\theta - p_Y sin\phi \tag{6}$$

where θ is the neutron scattering angle and ϕ is the nucleus recoil angle.
If particle Y is not observed which is usually the case, then ϕ and E_Y can be eliminated from the equations and a relationship between E_b and θ can be found.

$$E_b^{\frac{1}{2}} = \frac{(m_a m_b E_a)^{\frac{1}{2}} cos\theta \pm \{m_a m_b E_a cos^2\theta + (M_Y + m_b)[M_Y Q + (M_Y - m_a)E_a]\}^{\frac{1}{2}}}{M_Y + m_b} \tag{7}$$

This result is then used to sort the Geant4 events as elastic or inelastic scattering by using the Q value.

2. Simulation

To validate the performance of Geant4 in the implementation of primary neutron nuclear processes, a few conventional neutron scattering experiments were configured and simulated and the results were compared with the ENDF/B-VII database of cross sections.

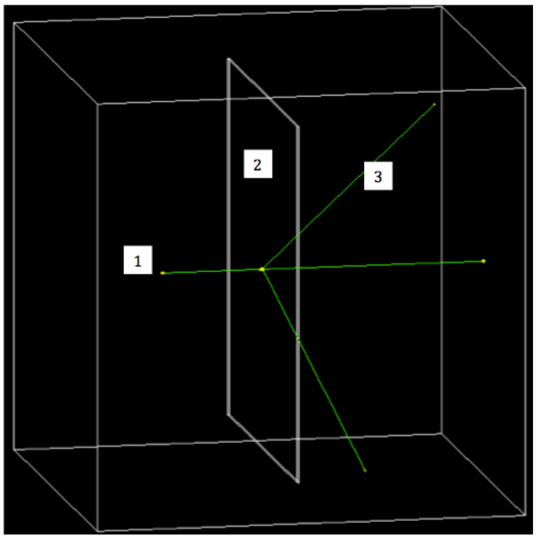

Figure 2. Illustration of the simulation of neutron scattering using Geant4. Point 1 represents a neutron generator; point 2 represents a target, which is one of the materials; point 3 represents neutron trajectories.

The simulation was a scattering experiment which consisted of a neutron beam that had randomly generated energies between 0 MeV and 10 MeV, and targets of three different well chosen materials with a thickness of 0.3 cm. The experiment was conducted in an empty box with the targets 10 cm away from the source. The target thickness was chosen in such a way as to avoid any secondary hard scattering events. The materials within which the neutron scattering was observed are Aluminium, Berylium and Carbon. In order to make a quantitative analysis of the simulation, current information of the incident particle needs to be accessible to the user. This, Geant4 makes viable via one or many of the useraction classes in the Geant4 kernel [5].

As an object oriented toolkit, a standard Geant4 simulation consists of the main program which is the executable. This main program is executed via the G4RunManager class, which controls the flow of the program and manages the event loop/loops within a run, and the G4UImanager class which creates a pointer to the interface manager, and allows the user to issue commands to the program [6]. The G4RunManager is also responsible for managing initialization procedures, including methods in the user initialization classes. A simulation program consists of some mandatory classes that are defined by the user, and these fall under the user initialisation classes and the useraction classes. The mandatory user initialisation classes are derived from the Geant4 base classes, .e.g. G4VUserDetectorConstruction from which the experimental setup is designed and the G4VUserPhysicsList wherein one can specify the kind of physics that is to take place between the target and the incident particles of choice. The mandatory useraction class is derived from the G4VUserPrimaryGeneratorAction base class, in this class one gives dynamic information about the incident particle. Other useraction classes that can be added to the main include the SteppingAction, TrackingAction, EventAction classes etc. In these classes the user can extract information about the track or event [2].

Geant4.9.5 was used together with a reference physics list called QGSP–BIC–HP, Quark-Gluon String–Precompound Binary–Cascade High–Precision model. This reference physics list is a high precision neutron package, NeutronHP for the transport of neutrons below 20 MeV down to thermal energies and is therefore the recommended physics list for low energy neutron physics [2]. A step is a single discrete movement of a particle and a track is a series of sequential steps that make up the history of the particle.The G4Step class, stores the transient information of a step. This includes the two endpoints of the step, PreStepPoint and PostStepPoint, which contain the points' coordinates and the volumes containing the points. G4Step also stores the change in track properties between the two points. These properties, such as energy and momentum, are updated as the various active processes are invoked [2]. Therefore information about the track was accessed via the SteppingAction class. The histograms were stored via the EventAction class, which stores collective information of an event.

3. Results and discussion

The results below show a comparison of the ENDF/B-VII cross sections with the the reconstructed cross sections obtained from the Geant4 simulation. Since the experimental configuration is a scattering one and the kinematics are typical neutron nuclear reaction kinematics, we were able to extract the elastic cross section by selecting those events which had obeyed the elastic scattering kinematics. This works, because for elastic reactions, the Q value, or the access energy is zero. However, it becomes cumbersome to determine the Q values of nonelastic reactions. One can also get the cross sections that Geant4 uses for a reaction directly from Geant4, by just requesting a cross section for that particular reaction. However the purpose of this simulation was not only to see which cross sections Geant4 is using, but rather to also determine how Geant4 implements the physics of these reactions. To get these results, the Geant4 kernel was used. In addition to the transient information of a step, the G4Step class has various other Get methods of accessing more information about a step. For these results the GetProcess and GetProcessType methods were used to get information about the kind of processes that took place at each step. An algorithm that sorted between the different hadronic processes that took place at each event was written and the histograms were populated by the incident energy thereby giving the cross sections.

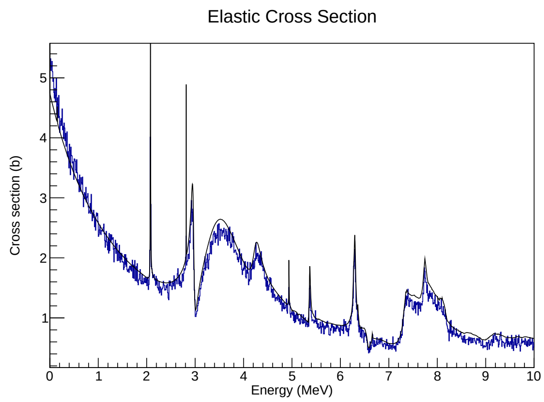

Figure 3. A comparison between ENDF/B-VII(Black) and Geant4(Blue) elastic cross sections of ^{12}C

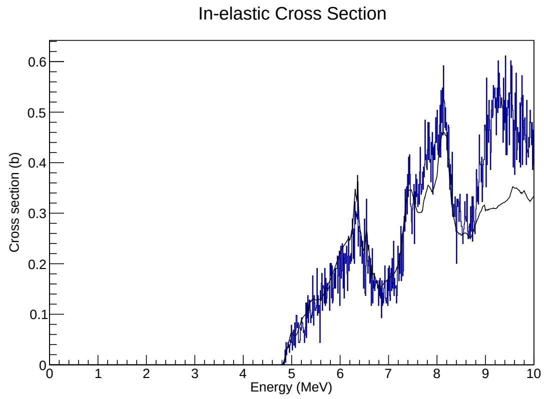

Figure 4. A comparison betweeen ENDF/B-VII(Black) and Geant4(Blue) inelastic cross sections of ^{12}C

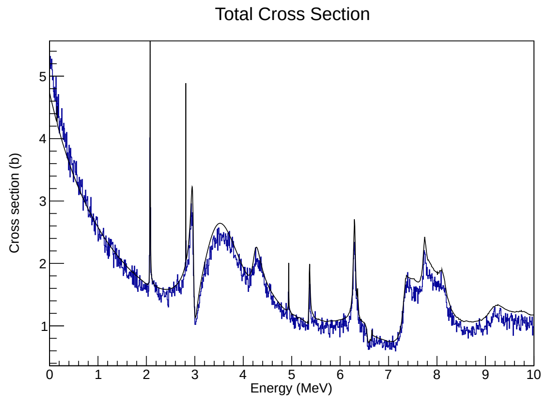

Figure 5. A comparison between ENDF/B-VII(Black) and Geant4(Blue) total cross sections of ^{12}C

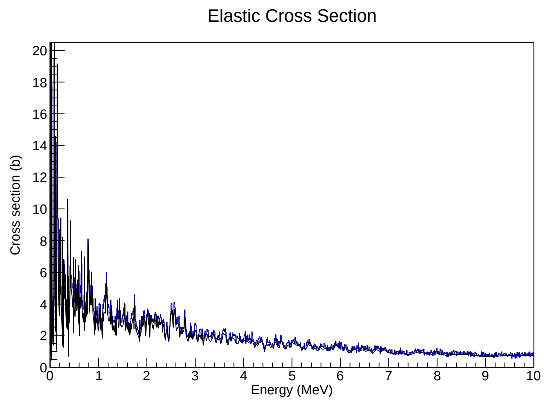

Figure 6. A comparison between ENDF/B-VII(Black) and Geant4(Blue) elastic cross sections of ^{27}Al

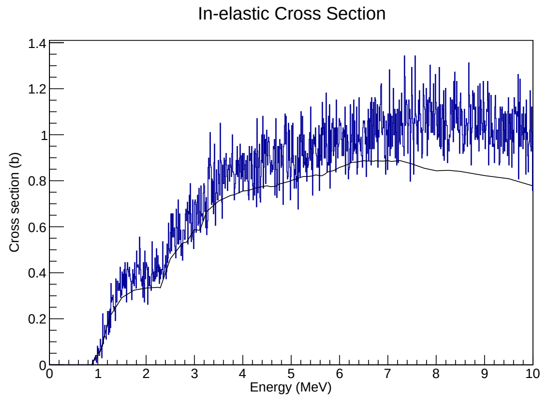

Figure 7. A comparison betweeen ENDF/B-VII(Black) and Geant4(Blue) inelastic cross sections of ^{27}Al

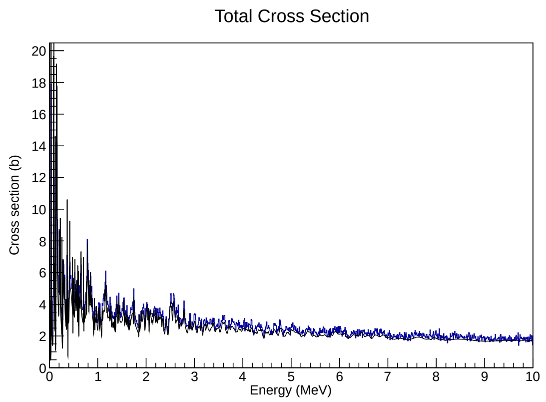

Figure 8. A comparison between ENDF/B-VII(Black) and Geant4(Blue) total cross sections of ^{27}Al

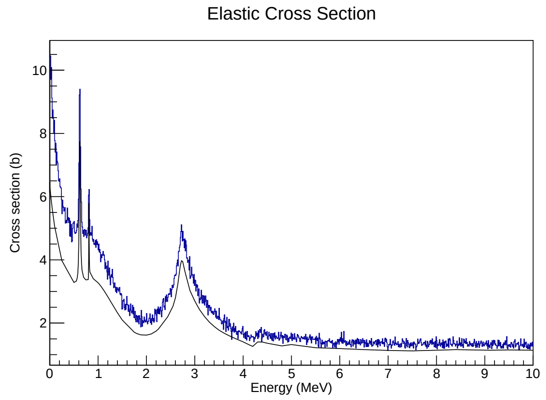

Figure 9. A comparison between ENDF/B-VII(Black) and Geant4(Blue) elastic cross sections of ^{9}Be

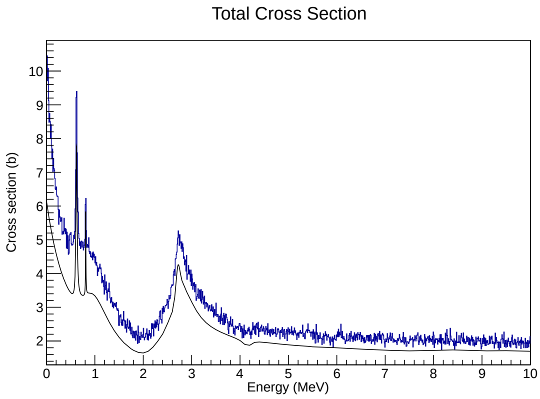

Figure 10. A comparison between ENDF/B-VII(Black) and Geant4(Blue) total cross sections of ^{9}Be

4. Conclusion

The histograms above show a fair correlation between the Geant4 cross section results and the ENDF/B-VII database cross sections. This partially validates the performance of Geant4 in the simulation of neutron induced reactions relevant to reactor studies. Although there are some inconsistencies in the absolute cross sections in terms of the scaling e.g Figure 10 and Figure 9 and some discrepancies at higher energies for the inelastic cross sections Figure 7 and Figure 4 the overall shape is fairly correlated. The discrepancies could be due to several issues. For example, there could be differences between the reference libraries and the libraries in this version of Geant4. There are also issues with the performance and configuration tuning of the neutron Physics Class [7]. These results are going to be a part of the continual investigation in the validation of Geant4 as a toolkit for reactor studies. There have been improvements [2] in the lower energy neutron physics in the latest version, Geant4 10.0 but those are yet to be tested.

5. References

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