A Comparison of Neutron Scattering in Geant4 and MCNP

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Abstract. Geant4 is a Monte Carlo based simulation tool that models the passage of particles through matter. It was developed at CERN primarily for High Energy Particle Physics. This research applied Geant4 in a simulation of single event neutron scattering in materials typical of the SAFARI reactor core. Four different materials were used in the simulation: Water, Aluminum(27), Uranium(238) and Beryllium(9). The results of the neutron scattering were compared with MCNPX2.7 results. This was done in order to validate the Geant4 implementation of primary processes within the ENDF/B-VII database of reaction cross sections and also benchmarking this against other simulation programs particular to low energy neutron transport like MCNPX 2.7. It was found that the Geant4 results compare well with MCNPX2.7 results. The total neutron scattering cross sections of Geant4 where also compared with the ENDF/B-VII cross sections and these also compared well.

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].

MCNP is a general-purpose Monte Carlo N-Particle code that is used for the transport of particles. The different areas of application are radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning [3].

The energy loss of neutrons is mainly due to elastic scattering, absorption and nuclear collisions[4]. A typical nuclear reaction is written as[5]:

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

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.

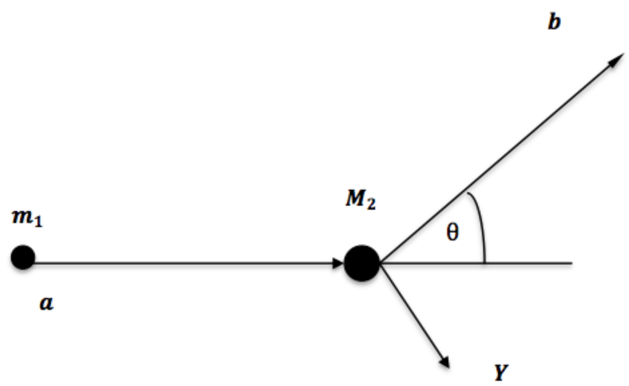

Figure 1. Kinematics of a nuclear reaction of the type a + X → Y + b

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. 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

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

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.

2. Simulation

To validate Geant4's implementation of primary processes within the ENDF/B-VII database of reaction cross sections a few simplistic experiments were simulated and the results were compared with MCNPX2.7 results. The Geant4 total neutron scattering cross sections were also calculated and compared with the ENDF/B-VII cross sections.

Four different well chosen reactor material targets with a thickness of 0.15cm were bombarded with a 5MeV Neutron beam. The simulation was run for 3600000 events. The target thickness was chosen to avoid any secondary hard scattering events. The materials within which the neutron scattering was observed are Aluminium, Uranium, Berylium and water. Histograms were populated by the energy of the exiting neutrons.

In the Geant4 platform the main program is implemented by two toolkit classes G4RunManager and GUImanager. The G4RunManager consists of subprograms three of which are mandatory. The mandatory classes are the initialization classes and the user action classes. These classes are G4VUserDetectorConstruction, G4VUserPhysicsList and G4VUserPrimaryGeneratorAction which are derived from the abstract base classes provided by Geant4. Other subprograms to 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. The G4UImanager creates a pointer to the interface manager. The manager class is created when the run manager is created. The User Interface is created in order for the user to issue commands to the program [6].

For the simulation, Geant4.9.5 was used. The track information was accessed via the SteppingAction class and the histograms are stored via the Event action class. 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].

In the MCNP platform the same setup was simulated. The simulation was ran for 15 minutes. This in MCNPX2.7 produces the same number of incident neutrons which is about 360000 source neutrons. The MCNPX2.7 code also produced histograms of the energies of the ejectile energy distributions.

3. Results and discussion

The graphs below show a good correlation between the MCNPX2.7 results and the Geant4 results. Although the scaling of the histograms is different, the number of particles with exit MeV are proportional in both the codes. Although the results are preliminary, it is assumed from the shape of the graphs that the scattering cross sections of Geant4 and MCNPX2.7 are similar.

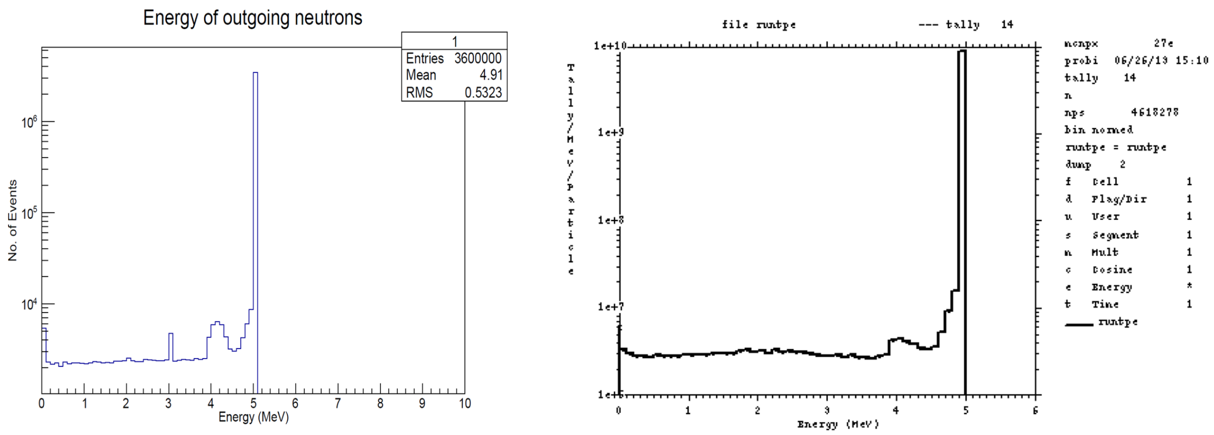

Figure 2. A comparison of neutron scattering in water in Geant4(left) and MCNPX(right).

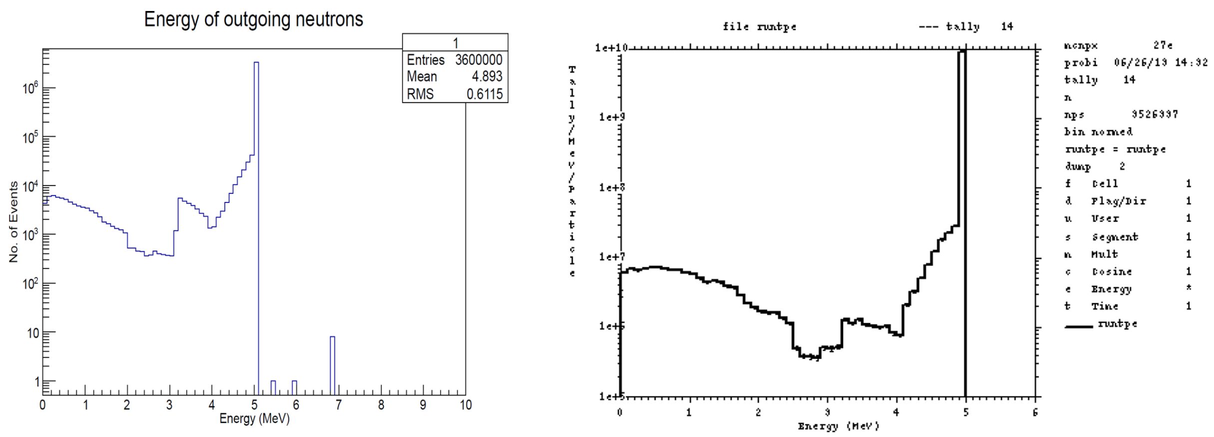

Figure 3. A comparison of neutron scattering in Beryllium in Geant4(left) and MCNP(right)

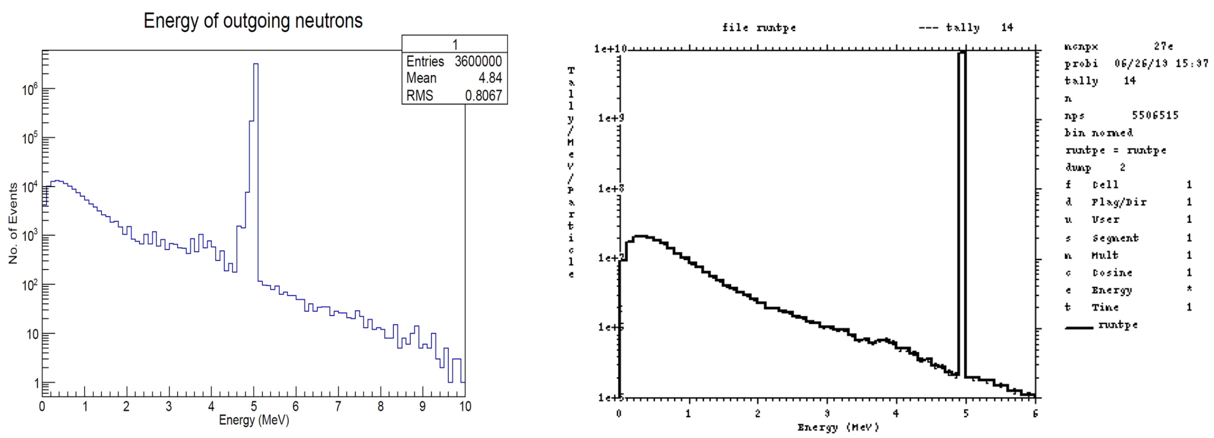

Figure 4. A comparison of neutron scattering in Uranium in Geant4(left) and MCNP(right)

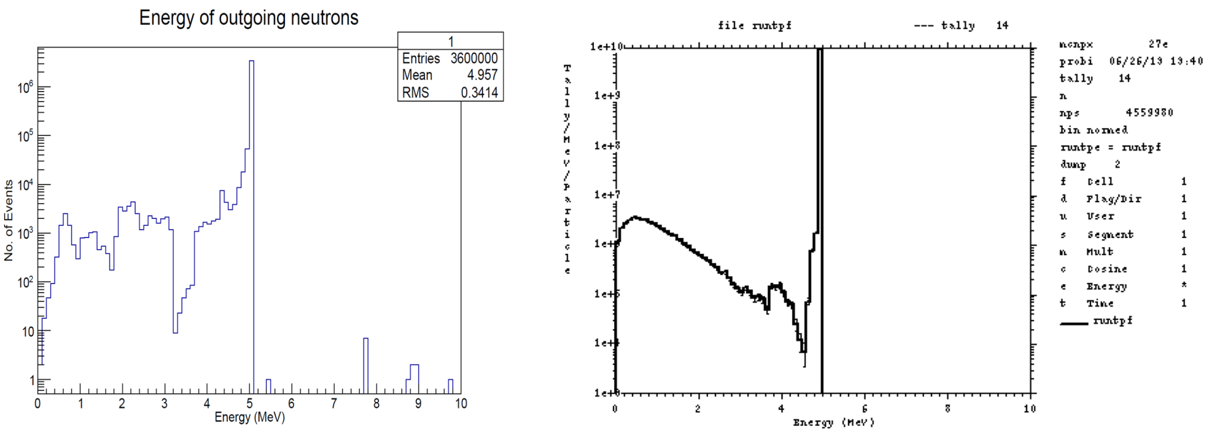

Figure 5. A comparison of neutron scattering in Aluminium in Geant4(left) and MCNP(right)

From the graphs we can see that most of the neutrons didn't interact with the target. Most of the events had an exit energy of 5MeV. This is a result of the choice of target thickness which insisted the interaction probability should be much less than one.

The Geant4 total neutron scattering cross section for Uranium(238), Carbon(12), Aluminium(27) and Beryllium(9) was calculated as follows [7]:

$$\sigma_{scat} = \frac{N_{scat}}{N_{tot}}\frac{1}{n_t} \tag{8}$$

where:

σ_{scat} = total cross section in barns

N_{scat} = the number of scattered neutrons

N_{tot} = total number of incident neutrons

n_t = surface density of the target calculated as follows :

$$n_t = \frac{\rho N_A}{M} t \tag{9}$$

Where:

ρ = Density of the target

N_A = Avogadro's number(6.022×10^{23})

M = Molar mass of the target

t = thickness of target(cm)

The Geant4 total cross section values are tabulated below:

Table 1. The comparison of Geant4 total scattering cross sections with ENDF/B-VII cross sections

Incident neutron energy	Material	Geant4	ENDF/B-VII	Error(σ)
5MeV	Uranium(238)	7.223 b	7.3646 b	3.223×10^{-2}
5MeV	Beryllium(9)	1.862 b	1.88691 b	2.628×10^{-2}
5MeV	Carbon(12)	1.177 b	1.18407 b	1.883×10^{-2}
5MeV	Aluminium(27)	2.323 b	2.3678 b	2.048×10^{-2}

The calculated total scattering cross sections are similar to the ENDF/B-VII cross sections. This validates the Geant4 use of ENDF/B-VII cross sections. The deviation in the calculated cross section value is due to a statistical error on the total number of scattered neutrons. The number of scattered of neutrons is described by a poisson distribution [4] therefore the error was calculated as $\sigma = \sqrt{N_{scat}}$.

4. References

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