

COMPARISON OF GEANT4 AND MCNPX FOR PROTON RADIATION TREATMENT SIMULATIONS

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ABSTRACT

GEANT4 and MCNPX are two codes that are frequently used to simulate proton radiation transport at MGH and RPI respectively. There has been no documented intercomparison of these two codes for the proton and secondary particles of interest to proton radiation treatment. This project compared dosimetric parameters obtained from these two codes for a water phantom slab. Results show that the energy distributions of protons coming out of the water slab are quite similar for the two codes in 150 MeV incident energy cases, while there are some discrepancies in the peak locations for the 100 MeV cases due to the problems in energy normalization. MCNPX predicts neutrons with, on average, higher energies than GEANT4. We believe this is due to the different physical models used for treating nuclear interactions by the two codes. Such information allows the users to validate certain dosimetric results that must be obtained from either code because of the resources currently available from these two popular codes for proton radiation treatment procedures.

Key Words: GEANT4, MCNPX, proton, radiation treatment

1 INTRODUCTION

Monte Carlo (MC) dose calculations are known to be more accurate than commercially available treatment planning system (TPS) that are based on fast but approximating semi-empirical algorithms for photons and electrons. Thus, the use of MC dose calculations in a TPS can lead to improved outcome in clinical photon and electron radiotherapy [1, 2]. In the field of proton radiation therapy, Monte Carlo simulations have also found widely applications such as calculating of neutron shielding requirements, verifying commercial pencil beam dose calculation models, and estimating the RBE in the patient [3].

Two popular Monte Carlo codes for proton radiation transport simulations are GEANT4 and MCNPX. GEANT4 is a Monte Carlo simulation toolkit based on object-oriented programming technology. The software has been developed through a collaboration of more than 100 scientists and was released in 1998 [4]. MCNPX is a 3-D Monte Carlo radiation transport code developed and maintained at Los Alamos National Laboratory capable of tracking 34 types of particle (including 4 light ions) at various energies [5]. The MCNPX code uses standard evaluated cross

section libraries, along with physics models for energy regions where cross section data are not available.

In a recent study, the photon and electron transport features in GEANT4 were compared against those from the MCNP, EGS4, and EGSnrc codes [6]. This study showed that results obtained from GEANT4 were comparable to those obtained using these other codes. It was concluded that the photon and electron physics of GEANT4 is valid. However, there has been no comparison of GEANT4 with other Monte Carlo codes for proton radiation treatment simulations.

It is important to study the nuclear interactions for proton radiation therapy. The reasons are three-fold [3]. First, the nuclear interactions contribute to ~20% of the total absorbed dose [7]. Second, these interactions may produce high-LET secondary particles, such as alpha particles, that have higher relative biological effectiveness (RBE). Last, the secondary neutrons can easily travel a long distance to deposit dose outside the target volume. The nuclear interaction models in GEANT4 have been evaluated at Massachusetts General Hospital (MGH) against a multiplayer Faraday cup measurement [3, 7]. The distribution of charge deposition was recorded for monoenergetic protons stopping in copper and carbon. Such a distribution includes two distinct regions, a build-up region and a sharp peak region. The build-up region is contributed entirely by protons stopping through nuclear interactions, while the latter entirely by (electromagnetic) EM interactions. In this way, the nuclear and EM process are completely separated in the measurement. Such a measurement supplied the required information to evaluate the nuclear interaction models in GEANT4 code. Inspired by this exploration, Mascia et al [8] did a similar evaluation work for MCNPX using the experimental data published by Paganetti and Gottschalk [3, 7].

It is also true, however, that the method described in the previous paragraph is a general global rather than a detailed check of the nuclear model. The results from such studies tell us whether the overall projected range distribution of charged secondary particles is correct, but it cannot check any particular reaction channel [3]. Differences in the predicted reaction channels will cause differences in the secondary particle yields as well as in their energy distributions. The objective of this paper is thus to study and compare the energy distributions of secondary particles generated from nuclear interactions using both GEANT4 and MCNPX.

2 METHODS AND MATERIAL

In the following sections, we first introduce GEANT4 and MCNPX codes. Simulations of proton ranges in the two codes are discussed including procedures to normalize the proton energies of the two codes. In the last section, the methods to calculate the energy spectra of secondary particles from nuclear interactions are discussed.

2.1 Monte Carlo Codes

2.1.1 GEANT4

Developed with advanced software-engineering technology, GEANT4 has many advantages over other general-purpose Monte Carlo codes. Instead of being a standalone executable, GEANT4 is a developing toolkit of C++ class libraries, covering various needs for solving

particle transport problems. A user of the GEANT4 code has to specify the detector geometry, physics processes, source particle, and specific user actions. The user must have intimate knowledge about programming, particle physics, and the Monte Carlo radiation transport theory. The benefit from these detailed processes in GEANT4 is its flexibility in dealing with various problems.

The original method in GEANT4 for transporting particles in CT-based voxels is unnecessarily slow. Some parts of the GEANT4 code were re-coded to improve the efficiency [9]. The modifications provide faster particle transport in CT voxels and quicker geometry optimization when geometry change occurs. More details about Monte Carlo dose calculation in the GEANT environment are given elsewhere [9].

2.1.2 MCNPX

MCNPX 2.4.k is a general purpose Monte Carlo radiation transport code that tracks all particles at all energies [5]. It is based on two Monte Carlo packages: Monte Carlo N-Particle (MCNP) and Los Alamos High-Energy Transport (LAHET). The code is an extension of MCNP to all particles and all energies, improvement of physics simulation models, extension of neutron, proton and photonuclear libraries to 150 MeV, and the formulation of new variance reduction and data analysis techniques. LAHET, on the other hand, is a modified version of High-Energy Transport (HETC) code and is capable of modeling the interactions of nucleons, pions, muons, light ions, and anti-nucleons by the geometry routines of MCNP [10]. LAHET brings the advantage of treating nuclear interactions above this cut-off energy with physical models, such as the Bertini or Isabel models. All these codes were developed at Los Alamos National Laboratory (LANL) and are distributed in the United States by the Radiation Safety Information Computational Center (RSICC) at ORNL.

2.2 Proton Ranges

Proton ranges calculated by the two codes may not be the same. The energies then need to be first normalized by the ranges for further comparisons. Specifically, we first simulated the Bragg curves in water for different monoenergetic proton energies from 70 to 250 MeV using these two codes respectively. Then, the depth of the distal 90% dose fall-off was calculated for each energy. Finally, a plot of MCNPX-energy vs. energy difference (MCNPX-GEANT4) was generated and fitted with a polynomial. The MCNPX energy was then changed so that it gives the GEANT4-range according to the fitted function.

Figure 1 shows the geometry used for the calculations of the proton range in MCNPX and GEANT4. A uniform broad proton parallel beam was modeled to incident perpendicularly on a semi-infinite water phantom. The detector is cylinder of 1-cm radius, segmented every 1 mm in depth. Proton doses to these small cylinder detectors were calculated. Separate simulations were run for each of the energies between 70 to 250 MeV, at a 10-MeV bin. Depth dose curve (Bragg curve) was plotted and the 90%-maximum-dose was calculated. Proton ranges were calculated by interpolating the two depths that neighbor the 90% dose point. Statistical uncertainties are about 1% at the plateau region.

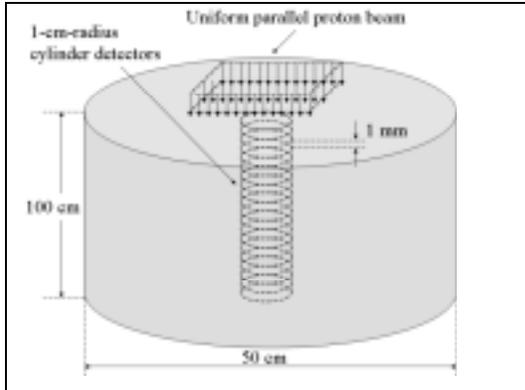


Figure 1. Geometry for calculating the proton ranges.

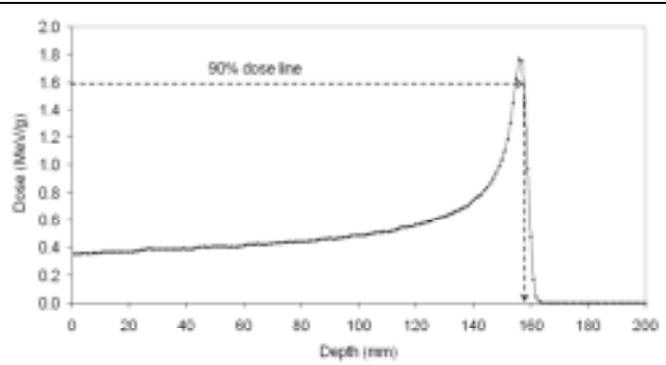


Figure 2. The simulated Bragg curve for incident protons of 150 MeV in the MCNPX code.

2.3 Particles Generated in Nuclear Interactions

We do not expect significant differences for electromagnetic interactions since the corresponding simulation physics is quite straightforward. On the contrary, the physical models for nuclear interactions are rather different. This is particularly important for studies on secondary radiation. To this end, secondary particles and their energy distributions were simulated and compared by the two codes.

In the simulations, a 1-cm thick water slab was placed in the vacuum. The water is used as a tissue equivalent material in the simulation. A point-like proton source was emitted in a single direction perpendicularly to the slab. The detector on the other side of the slab recorded the energy distributions of particles generated in nuclear interactions including neutrons, protons, alpha particles. The simulations were repeated for different energies between 100 MeV and 150 MeV.

3 RESULTS AND DISCUSSIONS

We first compare the proton ranges calculated by MCNPX and GEANT4, and then discuss the energy distributions for different particles coming out of a water phantom slab. MCNPX simulations were executed using a personal computer equipped with a 1.7-GHz CPU and 512-MB RAM under the Linux operating system. GEANT4 simulations were executed on a Linux cluster, built primarily with 38 2.2-GHz AMD CPUs.

3.1 Proton Ranges

In this section, we first present results on the Bragg curve. The proton ranges are determined from these Bragg curves in the energy range from 70 to 250 MeV. The ranges are then compared with the continuous-slowing-down approximation (CSDA) data from NIST. Finally, the polynomial fitting curve of energies is discussed in order to normalize the energies for MCNPX and GEANT4.

3.1.1 Bragg curves

In order to determine the proton range, Bragg curves were simulated in the energy range from 70 to 250 MeV in an interval of 10 MeV. Figure 2 shows such a Bragg curve for 150 MeV incident protons simulated by MCNPX. Based on this information, the proton range was then determined to be 157.55 mm using the approach described in previous sections.

The range of proton beams as simulated by GEANT4 was previously compared with measurements and excellent agreement within 1 mm was found for energies between 90 and 230 MeV [11].

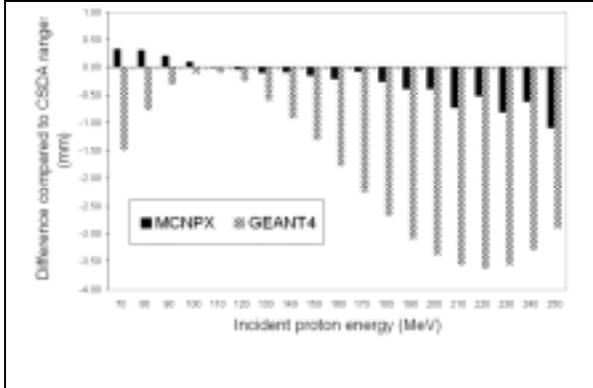


Figure 3. Proton range differences compared to CSDA range

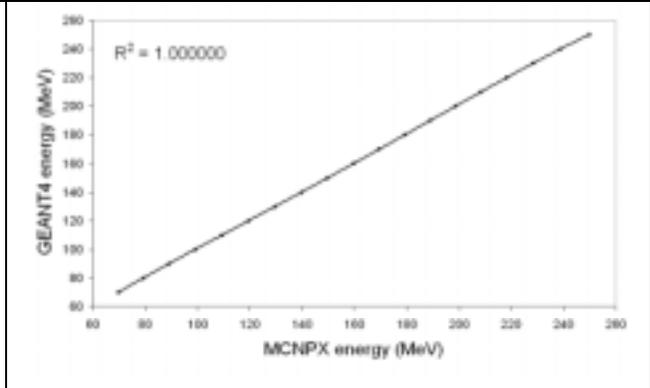


Figure 4. Polynomial fitting of energies for GEANT4 and MCNPX

3.1.2 Comparisons with CSDA

We also compared the calculated ranges with the CSDA data from NIST. CSDA is a very close approximation to the average path length traveled by a charged particle as it slows down to rest. In this approximation, the rate of energy loss at every point along the track is assumed to be equal to the total stopping power. Energy-loss fluctuations are neglected. The CSDA range is obtained by integrating the reciprocal of the total stopping power with respect to energy [12]. Even though there are differences between the definition of CSDA and our calculated ranges, the comparisons at least supply additional information on how accurate these calculated ranges are. As shown in Figure 3, GEANT4 always gives shorter ranges than the CSDA, while MCNPX only does so for energies higher than 100 MeV. Another observation is that the differences between the calculated and the CSDA are generally smaller for MCNPX than for GEANT4.

3.1.3 Polynomial fitting curve of energies

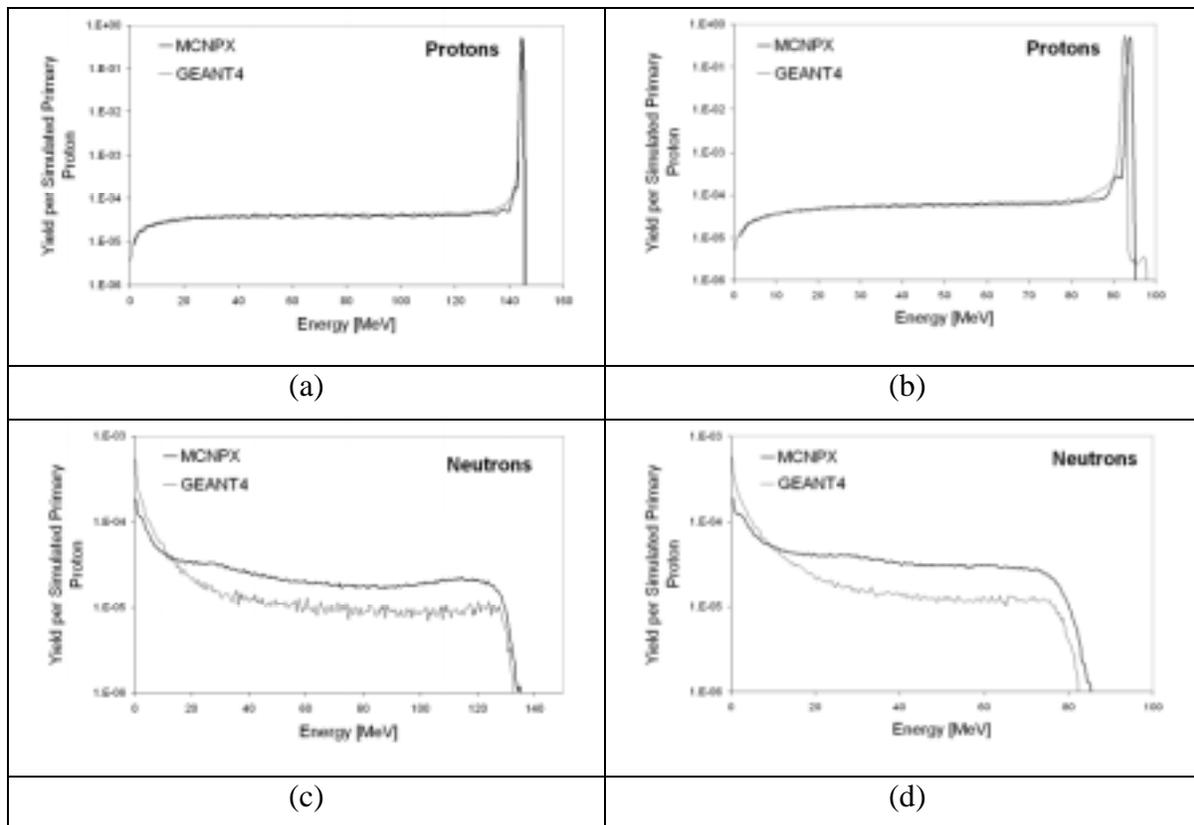
As explained earlier, proton ranges calculated by the two codes may not be the same and the energies need to be first normalized by the ranges for further comparisons. Figure 4 shows the polynomial fitting curve of energies for GENAT4 and MCNPX. The MCNPX energies were then changed so that they give the GEANT4-range according to this fit function. It is noted that the energies were only normalized from 70 to 250 MeV.

3.2 Energy Distributions for Particles Generated in Nuclear Interactions

The following results are based on 30 million histories for 150-MeV protons and 50 million histories for 100 MeV protons in GEANT4, respectively. On the other hand, 100 million

histories were simulated for both these energies in MCNPX. All the energy distributions were normalized per incident proton. Figure 5 shows the comparisons of the two codes for energy distribution of different particles coming out of a 1 cm of water phantom. The left panels present the results for 150 MeV incident protons, while the right panels for 100 MeV. As shown in Figure 5, the proton distributions are quite similar for 150 MeV incident energy cases, while there are some discrepancies in the peak locations for 100 MeV. It is believed to be caused by the energy normalization. MCNPX predicts neutrons with, on average, higher energies than GEANT4. We believe this is due to the different physical models used for treating nuclear interactions by the two codes. As for alphas, the results do not give much information. The statistical uncertainties are 30% or 40% for most of the points in the MCNPX curve and they are even worse for GEANT4 results due to smaller histories. However, most of the points of the two curves are still in the same magnitude regardless of such high statistical uncertainties. These results about alpha particles are qualitative rather than quantitative.

Another observation from these studies is that GEANT4 is more flexible than MCNPX in obtaining certain information on nuclear reactions. Besides the information given above, we can easily obtain other energy distributions from GEANT4 such as primary and secondary protons coming out of the slab, secondary protons and neutrons generated throughout the slab. On the other hand, such information cannot be as easily extracted from MCNPX.



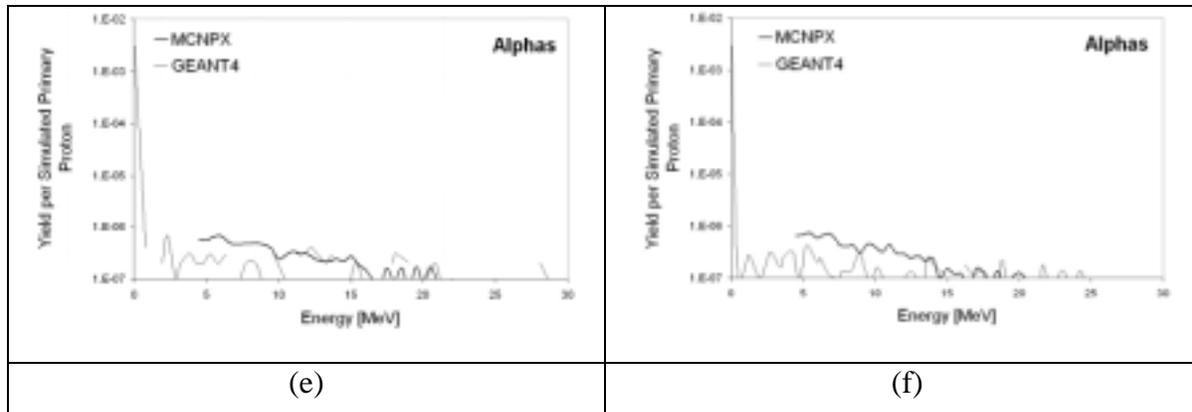


Figure 5. Comparison of particle spectra coming out of a water phantom. The left panels (a, c, e) present results for 150 MeV incident protons, while the right panels (b, d, f) for 100 MeV.

4 CONCLUSIONS

Two popular Monte Carlo codes GEANT4 and MCNPX for proton radiation therapy simulation have been compared in this study. The relevant nuclear physics was briefly reviewed. Two sets of results have been compared: proton ranges and energy spectra for different particles. Bragg curves are first calculated from the simulations and the proton ranges are then determined from these Bragg curves for each energy. These calculated ranges are then compared with the CSDA data from NIST. Finally, the energy distributions for different particles coming out of a water slab are discussed. For protons, the distributions calculated by the two codes are quite similar for 150 MeV incident energy cases. However, there are some discrepancies in the peak locations for the 100 MeV cases, which are believed due to the problems in energy normalization. MCNPX predicts neutrons with, on average, higher energies than GEANT4. We believe this is due to the different physical models used for treating nuclear interactions by the two codes.

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