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COMPARISON OF PARTICLE-TRACKING FEATURES IN GEANT4 AND MCNPX CODES FOR APPLICATIONS IN MAPPING OF PROTON RANGE UNCERTAINTY

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Abstract

The accuracy of proton therapy is partially limited by uncertainties that result from changing pathological conditions in the patient such as tumor motion and shrinkage. These uncertainties can be minimized with the help of a time-resolved range telescope. Monte Carlo methods can help improve the performance of range telescopes by tracking proton interactions on a particle-by-particle basis thus broadening our understanding on the behavior of protons within the patient and the detector. This paper compared the proton multiple coulomb scattering algorithms in the Monte Carlo codes MCNPX and Geant4 to well-established scattering theories. We focus only on beam energies associated with proton imaging. Despite slight discrepancies between scattering algorithms, both codes appear to be capable of providing useful particle-tracking information for applications such as the proton range telescope.

Keywords

Monte Carlo; proton imaging; multiple coulomb scattering

I. INTRODUCTION

Range uncertainties are manifest in proton therapy resulting from different pathological conditions such as shrinkage of the tumor and organ displacement associated with respiratory and cardiac motions.¹ During respiration, for example, the proton path length can vary as a function of time, as intervening organs such as the lung moves in and out of the proton beam. Since it is a tenet of radiotherapy to deliver the maximum amount of dose to the tumor volume while limiting the dose to adjacent normal tissue, a method to quantify such uncertainties in range becomes critical during proton therapy. One of the potential methods to monitor the range fluctuation in real time involves the so-called time-resolved range telescope. A complete appreciation of proton interactions that occur within the patient body and the range detection device will help improve the overall performance of the proton range telescope.

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Monte Carlo methods can be used to investigate the impact of proton interactions on the image quality of a proton range telescope. Monte Carlo codes are usually equipped with particle-tracking features that provide detailed information about the proton beam characteristics at any location in the user-defined geometry. This paper investigates the use of particle-tracking features in two well-known Monte Carlo codes: Geant4 version 9.0 and MCNPX version 5.0 (Refs. 2 and 3). In particular, we will evaluate the accuracy of the multiple coulomb scattering algorithms used in each Monte Carlo code by implementing these tracking features. Multiple scattering of protons within the patient body and the detector volume may significantly impact the image quality of proton range telescopes.

II. METHODS

The difference in proton physics modeling between Geant4 and MCNPX was tested by simulating proton pencil beams (idealized) of 235- and 335-MeV energies into $20 \times 20 \times 20$ cm of water in a water phantom. The particle-tracking features in both codes were utilized. The particle-tracking feature in the MCNPX code was activated using the PTRAC feature. The tracking feature in Geant4 was activated using an in-house phase-space generation code. As shown in Fig. 1 the beam characteristics (i.e., x , y , z , u , v , w , E) were recorded at the exit plane of the phantom. The scattering angle and displacement probability density functions (pdf's) were determined at the exit tracking plane T_1 as illustrated in Fig. 1. We consider only the upper 98% of the scattering angle pdf to validate a Gaussian approximation for this distribution thus avoiding the single-scattering Rutherford tail. By making use of the root-mean-squared (rms) scattering angles and displacements determined from these distributions, i.e., σ_y' and σ_y , beam ellipses at T_1 from MCNPX and Geant4 were computed and compared. Beam ellipses plot lateral displacement on the abscissa and the scattering angle on the ordinate for each particle. We can use properties of these ellipses as qualitative metrics for comparing the scattering properties of each code.

A second series of simulations was performed to investigate the potential impact of the different multiple coulomb scattering algorithms between MCNPX and Geant4 on image quality. For these simulations a 235-MeV proton pencil beam was sent through the same phantom used for the simulations discussed previously, but with an additional bone edge of density 1.85 g/cm^3 and 5-cm thickness, placed at the center of the phantom (see Fig. 1). An image was produced by mapping the water-equivalent path length (WEL) lost in the phantom for a given x and y position (defined by the image resolution) on tracking plane T_1 . The resolution of this image was set to $1 \times 1 \text{ mm}$. The differences in image contrast between the two simulations were assessed.

III. RESULTS

Figure 2a compares the scattering angle pdf's taken at T_1 between MCNPX and Geant4 for a 235-MeV proton pencil beam that has traversed through 20 cm of water (see Fig. 1). Also provided in Fig. 2a are pdf's produced from the multiple scattering theories of Moliere, Highland, and Rossi.⁴⁻⁶ All theoretical values were calculated using an in-house software called LOOKUP developed by Gottschalk.⁷ The MCNPX results agree well with Rossi but overestimate σ_y' compared to the theories of Moliere and Highland. The agreement with Rossi is expected since the multiple scattering algorithm in MCNPX is derived from the Rossi formalism. Geant4 underestimates σ_y' compared to the theories of Moliere and Highland but is in better agreement with theory compared to MCNPX. The Geant4 multiple scattering algorithm is derived from a modified Highland formula. Figure 2b compares the lateral displacement pdf's taken at T_1 between the two codes for the same beam energy and geometry. As seen in Fig. 2b, MCNPX is slightly more accurate at estimating σ_y than Geant4 at calculating the lateral displacement of the proton beam compared to our

theoretical calculation using Highland's formula for $\sigma_{y'}$. Figure 2c compares the phase-space diagrams produced at T_1 between MCNPX and Geant4. Figures 2d and 2e provide the same plots as Figs. 2a, 2b, and 2c but for a proton beam energy of 335 MeV. Similar to the 235-MeV proton beam results, MCNPX overestimates $\sigma_{y'}$ and Geant4 underestimates $\sigma_{y'}$ compared to the theories of Moliere and Highland. However, the discrepancies are smaller, suggesting that both codes become more accurate at higher energies. Table I summarizes the results of these comparisons. It is interesting to note that along with Gottschalk⁸ we noticed a step size effect on our scattering and displacement distributions. The results presented below were generated using the default step size set in Geant4. We would also like to mention that tracking recoils in MCNPX by evoking the seventh entry on the PHYS:H card did not impact $\sigma_{y'}$ or σ_y .

Figure 3 provides the results of the simulations to study the impact of disparities in the scattering algorithms between MCNPX and Geant4. Figures 3a and 3b plot the projected WEL images at T_1 produced by MCNPX and Geant4. We plot only the protons within 7.0 mm of the beam axis, which was chosen to reflect 98% of the protons that fall within the Gaussian approximation of the displacement distribution. Figure 3c shows a profile taken at the center of the image plane to show the differences in contrast between the images. As shown, the differences in scattering algorithms between the two codes do not significantly impact the image contrast for this simple case. For Geant4 the water/bone contrast at the center of the image plane was calculated to be 2.16% whereas the MCNPX water/bone contrast ratio was calculated to be 2.43%.

IV. SUMMARY

This project showed that both MCNPX and Geant4 are capable of providing particle-tracking information for applications such as the proton range telescope. However, there appear to be slight discrepancies in the multiple coulomb scattering algorithms used between the two codes resulting in different $\sigma_{y'}$ and σ_y values calculated by our simulations. Based on the result of this study, Geant4 is more accurate at calculating $\sigma_{y'}$ whereas MCNPX is more accurate at calculating σ_y when compared to the theories of Moliere and Highland. However, we were able to show that these discrepancies may not impact the quality of the images produced by the two codes. The scattering and displacement distributions need to be fully assessed in more complicated geometries to fully appreciate uncertainties due to code-specific algorithms in the context of time-resolved range telescope simulations.

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Fig. 1.

Geometry definition used for comparison, showing idealized pencil beam entering the tracking devices and phantom. Shown in red is the bone slab that was placed within the water phantom for our image quality calculations (color online only).

Fig. 2. Comparison of scattering algorithms between MCNPX and Geant4. Figures (a), (b), and (c) are for a 235-MeV beam, and Figs. (d), (e) and (f) are for a 335-MeV beam. Figure (a) compares the scattering angle pdf's taken at T_1 between MCNPX and Geant4. Figure (b) compares the displacement pdf's taken at T_1 between MCNPX and Geant4. Figure 3c compares the phase-space diagrams produced at T_1 between MCNPX and Geant4. Figures (d), (e), and (f) are the same as Figs, (a), (b), and (c) but for the 335-MeV beam.

Fig. 3.

Impact of differences in multiple coulomb scattering models on image quality using a simple phantom. (a) WEL image generated using MCNPX. (b) WEL image generated using Geant4. (c) A profile demonstrating the contrast for these images for both codes. The WEL was calculated by the power-law formula $R(E) \cong aE^b$, where $a = 0.0022$ and $b = 1.77$, assuming R is in centimeters and E is in mega-electron-volts.

TABLE I

Comparison of the rms Scattering Angle $\sigma_{y'}$ and Displacement σ_y Between Monte Carlo and Theory for Geant4 and MCNPX*

	$\sigma_{y'} \text{ (deg)}$	$\sigma_y \text{ (cm)}$	$(\sigma_{y'}/\sigma'_{Theory} - 1)$	$(\sigma_y/\sigma_{Theory}^{-1})$
235 MeV				
Geant4	1.596	0.279	-0.043	-0.094
MCNPX	1.909	0.323	0.144	0.049
335 MeV				
Geant4	1.036	0.193	-0.033	-0.094
MCNPX	1.216	0.210	0.134	-0.014

* σ'_{Theory} was calculated directly by the theory of Moliere. σ_{Theory} was calculated directly using the theory of Highland to calculate $\sigma_{y'}$.