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Comparison of MCNPX and Geant4 proton energy deposition predictions for clinical use

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Abstract

Several different Monte Carlo codes are currently being used at proton therapy centers to improve upon dose predictions over standard methods using analytical or semi-empirical dose algorithms. There is a need to better ascertain the differences between proton dose predictions from different available Monte Carlo codes. In this investigation Geant4 and MCNPX, the two most-utilized Monte Carlo codes for proton therapy applications, were used to predict energy deposition distributions in a variety of geometries, comprising simple water phantoms, water phantoms with complex inserts and in a voxelized geometry based on clinical CT data. The gamma analysis was used to evaluate the differences of the predictions between the codes. The results show that in the all cases the agreement was better than clinical acceptance criteria.

Keywords

Monte Carlo validation; Geant4; MCNPX

1) Introduction

Proton therapy in patients with cancer is an evolving treatment modality that affords many advantages due to the particular shape of the dose distributions (Bragg peaks) achievable with heavy charged particles. Many studies have been performed to demonstrate the advantages of this treatment modality; however, to fully exploit them, many challenges must still be overcome. The latest development, intensity-modulated proton therapy, is expected to provide dose distributions that are superior even to conventional, passively scattered proton therapy (Zenklusen *et al.*, 2011; Soukup *et al.*, 2009; Thorwarth *et al.*, 2008; Oelfke and Bortfeld, 2003; Lomax, 2008b, a; Timmermann *et al.*, 2007; Tourovsky *et al.*, 2005; Lomax *et al.*, 2004; Pedroni *et al.*, 1995). But, as usual, progress has a price. With IMPT, the complexity of the dose delivery once more increases and more complex treatment plans have to be developed. Current proton treatment planning software, relying on semi-empirical or analytical dose prediction algorithms are pushed to the limits by the complexity of these problems. Heterogeneities with large density gradients, such as metallic implants or complex air-bone-interfaces, represent cases in which the physics of charged particle transport is much more unforgiving than that of photon transport. In these cases, multiple Coulomb scattering and inelastic scattering of primary particles, as well as range straggling and a multitude of nuclear interactions of the charged projectiles with target nuclei pose substantial challenges to analytical or semi-empirical dose prediction algorithms.

For these reasons, many proton therapy centers compute dose distributions using the Monte Carlo method. Monte Carlo simulations are commonly assumed to provide the most accurate dose predictions, because they are based on first principles. Some institutions have created their own, “in-house” Monte Carlo codes (PSI, Switzerland) for dose prediction in such complex cases, however, there are also several well-known general purpose Monte Carlo packages available which are popular among medical physicists, among the most prominent of which are the Geant4 code (Agostinelli *et al.*, 2003; Allison *et al.*, 2006) and the MCNPX code (Waters *et al.*, 2005). Geant4 is an object-oriented Monte Carlo toolkit originally developed at CERN. Currently, the code is maintained by the Geant4 collaboration, which is an international concert of scientist and software engineers whose goal is to develop, maintain and provide support for the toolkit. Geant4 has been utilized for high energy, nuclear and accelerator physics applications, as well as studies in medical and space science. MCNPX is a development by the Los Alamos National Laboratories (LANL) and constitutes one of the gold standards of radiation transport simulations. Its development started in 1947 and is still ongoing.

These simulation programs have been adapted and validated (Paganetti and Gottschalk, 2003; Paganetti *et al.*, 2004; Newhauser *et al.*, 2007; Polf *et al.*, 2007; Bues *et al.*, 2005; Newhauser *et al.*, 2005; Sawakuchi *et al.*; Titt *et al.*, 2008) by the proton therapy centers at the Massachusetts General Hospital (MGH, Boston MA) and at the University of Texas M.D. Anderson Cancer Center (MDACC, Houston TX), to provide, what is commonly perceived as “the most accurate” dose prediction achievable. While Monte Carlo codes simulate radiation transport based on first principles, good accuracy can be expected, however users of Monte Carlo systems can choose between many physics models (such as intra-nuclear cascade physics, multiple Coulomb scattering, etc...) for particular tasks, which may influence the results (Zacharatou Jarlskog and Paganetti, 2008).

Hence, a collaborative study was performed to estimate the discrepancies amongst different Monte Carlo systems by evaluating the differences between the energy deposition predictions from Geant4 and MCNPX. The purpose of this study is to evaluate the two Monte Carlo codes employed for proton dose predictions in a variety of cases including simple and complex phantoms as well as a patient geometry based on computer tomography (CT) images. Monoenergetic proton beams of 100 and 200 MeV, as well as a spread out Bragg peak (SOBP) with a range in water of 17.2 cm and a modulation width of 5.0 cm (distal 90% to proximal 90%) were simulated. Lateral and longitudinal energy deposition profiles were scored and compared and analyzed with the Gamma method (Low *et al.*, 1998). The results of the study provide a conservative estimate of the achievable accuracy using either MCNPX or Geant4, because all simulations were performed using the most basic code setups and as many default parameters as possible.

2) Methods and Materials

2.1) Codes

Two Monte Carlo codes were employed to predict energy deposition from proton beams in this study: Geant4 version 9.0 and MCNPX version 2.6. Particle transport in both codes can be performed using either a combination of tabulated cross sections and modeled data or modeled cross section throughout the entire particle energy range. The tabulated data is generally considered more accurate; however model calculations were used exclusively, to provide the “worst case scenario”. The implemented problem geometries were identical for both sets of simulations and are described in detail in section 2.2. The physics options chosen and the tally choices for the simulations are given in sections 2.3 and 2.4, and a detailed description of the implemented materials is given in section 2.5.

2.3) Physics

2.3.1) MCNPX—The simulations were performed with as many as possible default parameters in MCNPX, while the Geant4 code was configured using parameters described in section 2.3.2 and the references within. In both systems, primary and secondary protons, as well as secondary neutrons, photons, electrons, deuterons, tritons, alpha particles and heavy ions were transported. For the protons, as for all other particles transported in the simulations, the maximum transport energy was set to 205 MeV. The analog energy limit, above which the system would simulate implicit capture, was set to 0 MeV. Table based physics was disabled, so only physics models would be used. Furthermore, charged particle straggling was treated with the Vavilov-model and light ion recoil from elastic scattering was enabled. The neutron physics used a 0 MeV analog energy limit to enable implicit capture, the control of unresolved resonances was set to ON. Again the table based physics was disabled, fission multiplicity was set to 0 and ion recoil was enabled, and neutron capture ions were created. In the photon physics the electron production was turned on, coherent scattering (Thomson scattering) was enabled, photonuclear particle production was disabled, Doppler energy broadening and delayed gamma production were disabled. Electron physics used bremsstrahlung production, photon creation was turned ON, the bremsstrahlung angular distribution was performed using the full bremsstrahlung tabular angular distribution, energy straggling was based on sampled straggling for energy loss, and the number of bremsstrahlung photon multiplicity was 1. Furthermore, the production of electron-induced x-rays was set to 1, knock-on electron multiplicity also was set to 1 and finally, analog bremsstrahlung production was enabled. Finally, for the heavy ions the energy straggling was treated according to Vavilov (Vavilov, 1957).

For all transported particles the cutoff energy, at which the transport would be terminated and the remaining kinetic energy deposited locally was set to 0, to force the use of the minimum available energy cutoff values. For all particles this value is 0.001 MeV except for neutrons. Neutron transport cutoff energy was 0 MeV (capture or escape from the geometry).

2.3.2) Geant4—Similarly, primary protons and secondary protons, neutrons, photons, electrons, deuterons, tritons, alpha particles and heavy ions were transported during the Geant4 simulations. All relevant physic processes were initiated for the simulations. The standard electromagnetic physics package was used to model multiple Coulomb scattering and ionization for charged particles. Inelastic processes were handled using the low energy ionic and Binary Cascade models. The Geant4 binary cascade model propagates primary and secondary particles in a nucleus via an intranuclear cascade, where interactions take place between a primary or a secondary and an individual nucleon in the nucleus. The low energy electromagnetic hadronic model was employed for the energy loss calculations. For protons, we set a range cut-off of 0.05 mm for the secondary production threshold. All other physics settings are reported elsewhere (Jarlskog and Paganetti, 2008).

2.4) Tallies

The energy deposition per volume, in units of MeV cm^{-3} , was scored in both Monte Carlo systems and compared using the Gamma analysis method. The MCNPX code utilized a mesh tally type 3 (total energy deposition from primary and secondary particles). The setup consisted of a rectangular mesh with a 1 mm spatial resolution in the direction of the lateral profiles, 50 mm perpendicular to the profiles and 10 mm in depth, as well as two circular mesh tallies with a one mm resolution in beam direction, using radii of 1 cm and 10 cm respectively. For the Geant4 simulation, user-defined histograms were used to score energy deposition events using the histogram package known as AIDA. The boundaries on the histograms were set to reflect the exact same tally geometry employed for the MCNPX

simulations (i.e. both the rectangular and cylindrical mesh). Please note that the energy deposition per volume in water is proportional to dose because the density of water was assumed to be 1 g cm^{-3} .

2.5) Materials

Materials included in the phantom setups consisted of air, bone (photon bone equivalent), lung (photon lung equivalent), brass and water and are described in detail in Table 1. Additional materials had to be implemented for the use of the voxelized patient geometry based on CT images. In order to utilize CT data in a Monte Carlo geometry, one has to convert the Hounsfield units (HU) from the CT into material and density combinations, which are then implemented in the voxels constituting the patient geometry in the simulations. The HU conversion methods employed were different, according to the methods used at the respective treatment facilities. MGH used an algorithm based on Schneider et al (Schneider *et al.*, 2000) while MDACC employed a method published by Schneider et al (Schneider *et al.*, 1996). Both methods require grouping together different tissues (i.e. HU numbers) sharing the same material composition and mean ionization potential. For the Geant4 simulations, the HU space was divided into 27 groups: 1 group for air, 1 group for lung tissue, 7 groups for soft tissue, 15 groups for skeletal tissues and 3 groups for high-Z materials. However, each individual HU number had a unique density assigned to it. This is slightly different than the MCNPX implementation where air too was 1 group, 14 different soft tissues were implemented, and 10 groups for skeletal tissues were used. The densities were varied inside each group, depending on the HU value from the CT data.

2.6) Geometry (Geant4 and MCNPX)

Several different geometries were simulated during this study. The simplest case consisted of the dose scored in a cubic water phantom. An 8 cm thick brass collimator with a $10 \times 10 \text{ cm}^2$ aperture, located with the downstream surface at a distance of 10 cm to the upstream surface of the water phantom. The phantom had a size of $50 \times 50 \times 50 \text{ cm}^3$. The density of the water was assumed to be 1 g cm^{-3} ; the density of the brass was set to 8.38 g cm^{-3} . No walls around the water phantom were considered. The phantom and the brass collimator were encased in an air space that had a nominal density of 0.0012 g cm^{-3} . Next, half beam blocks (HBBs) of lung tissue or of bone material, with a lateral extend of $5 \text{ cm} \times 10 \text{ cm}$ and a thickness of 8 cm were inserted into the aperture to compare stopping power and scattering performance. The lung tissue density was assumed to be 0.25 g cm^{-3} , and the bone tissue was simulated with a density of 1.85 g cm^{-3} . The stoichiometric composition of the materials was taken from ICRU 44 (ICRU, 1989) and can be found in table 1, in section 2.5. A more complex phantom consisted of a water phantom containing three solid cylinders of bone material with 2 cm diameters, located with the central axis of the cylinder at a depth of 3 cm in the phantom. The cylinders were oriented perpendicular to the beam direction. Furthermore, a slab of lung material (4cm thick) was located directly downstream of the bone cylinders. Finally, the phantom was replaced with an anonymized, voxelized geometry of a head and neck cancer patient, based on CT images. The voxelized volume was located such that the "patient" would receive a "left lateral" beam and the isocenter was located just superior to the larynx.

The starting positions of the source particles were randomly sampled on a plane located at the upstream surface of the brass collimator. The lateral extend was $10 \text{ cm} \times 10 \text{ cm}$, matching the aperture size. Source protons were monoenergetic (100 MeV or 200 MeV respectively) and their initial direction was along the z -direction (beam axis). Simulations using an SOBPs were performed by reading the directional cosines and the kinetic energy of the source particles from a file (so called "phase space"), created during the simulation of a

proton beam passing through the entire treatment head geometry at the MGH (Paganetti *et al.*, 2004), exhibiting a nominal range in water of 17.2 cm and a nominal modulation width (proximal 90% to distal 90% location) of 5.0 cm. Table 2 lists all beam parameters and phantom geometries, which were used in the comparison of Geant4 and MCNPX simulations.

3) Results

3.1) Lateral and longitudinal energy deposition profiles in phantoms

Lateral profiles were scored at depths of 5, 10, 15, 20, and 25 cm in the phantom. The resolution of the scoring tally was $1 \times 50 \times 10$ mm. Longitudinal profiles (in beam direction) were scored in two circular tallies with radii of 1 cm and 10 cm respectively and a resolution of 1 mm in beam direction. The profiles produced by MCNPX were compared to the ones produced by Geant4 by application of the Gamma analysis method, using failure criteria of 1 mm distance to agreement and 1% (of the maximum energy deposition) difference, 2mm and 2% and finally 3mm and 3%. In order to avoid biased results by comparing low energy deposition bins distal to the peak, we limited the analysis to the region of the beam entrance, the peak, and energy depositions 2 cm distal to the Bragg peak. Examples of these profiles and the corresponding gamma analysis are shown in Figure 1. Figure 1a shows the longitudinal energy deposition profile (corresponding to a depth dose profile) of a 200 MeV proton beam through an 8 cm thick HBB made of lung tissue with a density of 0.25 g cm^{-3} . Figure 1b shows the Gamma analysis of the comparison of these profiles for three different acceptance criteria. Data points with a Gamma index ≤ 1 would be accepted. In Figure 1c, the lateral energy deposition profiles at a depth of 15 cm in the water phantom are displayed, and finally in Figure 1d) the Gamma analysis of these profiles are displayed.

3.2) Energy deposition in the complex phantom

Longitudinal energy deposition profiles, and lateral energy deposition profiles of a monoenergetic proton beam (100 MeV) in the complex phantom, containing bone cylinders and a lung slab are shown in Figure 2. The results of the Gamma analysis are presented as well. Please note that the longitudinal energy deposition shows low values in the region where the lung slab was located, because the energy deposition was scored in units of MeV cm^{-3} per source particle.

3.3) Energy deposition distributions in the CT geometry

Two dimensional energy deposition distributions of the energy deposition from a monoenergetic proton beam of 100 MeV inside the CT phantom were scored with two-dimensional tallies with a spatial resolution of $0.976 \times 0.976 \times 3 \text{ mm}^3$, corresponding to the CT voxel size. Here too, the gamma analysis was applied, using criteria of 1%–1mm, 2%–2mm, and 3%–3mm. Again, to avoid biasing the results, only the high energy deposition areas and a margin of 2 cm of the low energy deposition region (i.e., outside the field) were included in the analysis. Figure 3 shows the results of the 2%–2mm-Gamma analysis of the comparison of the simulation data in the coronal plane.

3.4) Summary of gamma analysis

Finally, the statistics of all Gamma analysis results were evaluated. Figure 4 shows the distribution of the results from the gamma resolution for all lateral profile of the cases investigated. Figure 5 shows the results for the longitudinal profiles, as well as for all two-dimensional energy deposition distributions investigated in water phantoms. The lateral profiles of all phantom simulations, including simple water phantoms, HBBs, and the complex phantoms, were evaluated at depths of 5 cm, 10 cm, 15 cm and 25 cm. The mean

3%–3mm agreement was in all cases larger than 95%. The mean 2%–2mm agreement was >95% at 5 cm depth, >90% at 10 cm depth, >93% at 15 cm depth and about 88% at a depth of 20 cm. The best 1%–1mm agreement was achieved at a depth of 5 cm, showing 78.5 %. The worst case was 1%–1mm at a depth of 20 cm with only about 56% agreement. The depth doses from these simulations showed slightly better results, as for 3%–3mm the agreement was more than 96% in all cases investigated. The 2%–2mm analysis yielded >92%, and the 1%–1mm results agreement was about 83%. Comparison of two dimensional energy deposition distributions of phantom simulations using the gamma evaluation method yielded about 98.5% for 3%–3mm, about 95% for 2%–2mm, and a mean value of >73% using the 1%–1mm criteria. The gamma analysis performed on the simulations in the CT geometry yielded about 99% agreement for 3%–3mm, about 96% for 2%–2mm, and about 75% for the 1%–1mm criteria.

3.5) Uncertainties

In all cases the relative statistical uncertainties (1σ) of the results were recorded and evaluated. The best relative uncertainties were achieved with high energy proton beam simulations in simple water phantoms and were typically on the order of 1%. In all other simulations relative statistical uncertainties were kept below 3% in the high energy deposition region, which was the worst case, recorded in the proton beam simulations in the CT geometry. An example of the uncertainty distribution in a water phantom simulation with a lung material HBB is shown in Figure 6.

4) Discussion

The statistics of the results from the gamma analysis of a wide range of simulation data suggests that even in a situation using no sophisticated optimization of any physics parameters in either Monte Carlo system, a very good agreement between Geant4 and MCNPX can be achieved. At the M. D. Anderson Cancer Center, quality assurance of routine IMRT treatments with photons and IMPT treatments with protons are expected to yield >90% agreement for 3%–3mm criteria in the gamma analysis. The Monte Carlo result comparison showed much better agreement in almost all cases. The worst comparison using 3%–3mm limits were encountered in the lateral profile comparisons at a depth of 10 cm in the phantom, where the lowest percentage of agreement was found by comparing low energy beams in a complex phantom, i.e., where large energy deposition gradients were encountered. The 2%–2mm and 1%–1mm comparisons show expectedly worse results because of further introduction of small differences by the increased complexity of the geometry. However, even in stereotactic radiosurgery, where quality assurance standards are more stringent, a 3%–3mm agreement of 95% would be accepted. Again the comparison of Geant4 and MCNPX showed better agreement in all geometries considered in this study.

Comparing both codes with measured data is not as straight forward as it may seem. In order to do a deeper analysis, detailed models of both treatment heads would be needed in at least one of the Monte Carlo codes. However, the treatment head at the MDACC is modeled in MCNPX only whereas the MGH treatment head is modeled solely in Geant4.

In summary, the default configurations of the MCNPX Monte Carlo code and the configuration of Geant4 as described in 2.3.2 lead to energy distributions patterns that compare within limits which achieve or are superior to the clinically used quality assurance criteria.

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Figure 1.
Example longitudinal and lateral energy deposition profiles calculated with Geant4 and with MCNPX, also showing the respective results of the Gamma analysis.

Figure 2.

Lateral and longitudinal energy deposition profiles in the complex phantom geometry. The lateral profiles shown in Figures 2a and 2c, as well as the longitudinal profiles (Figure 2e) show excellent agreement, as can be seen from the Gamma index analysis data given in Figure 2b, d and f.

Figure 3. Example of results of the dose prediction in a coronal slice of the CT geometry using (a.) MCNPX and (b.) Geant4 (values in MeV cm^{-3} per source particle). (c.) 2D Gamma analysis of energy deposition in a CT geometry representing a patient. Acceptance criteria were 2% and 2 mm in this case. White points were those with $\Gamma > 1$, i.e., points which failed. The CT image indicates the field size and direction of the proton beams.

Figure 4. Statistics of Gamma analysis results of the lateral profile comparisons at various depths for all water phantom cases investigated.

Figure 5. Statistics of Gamma analysis results of the longitudinal energy deposition profile comparisons of all water phantom cases.

Figure 6. Example of relative uncertainties, σ , of the 200 MeV proton simulation through an 8cm thick HBB, consistent of lung material, in a simple water phantom.

Table 1

materials implemented in the phantom setups and part of the patient geometry setup, excluding the voxelized patient geometry. The parameters listed here were identical in MCNPX and Geant4.

Material	Element	Weight %
Air	C	0.000124
	N	0.755266
	O	0.231786
	Ar	0.012824
Water	H	0.111907
	O	0.888093
Brass	Fe	0.00001
	Cu	0.605379
	Zn	0.394591
	Pb	0.00002
Bone (compact)	H	0.063984
	C	0.278
	N	0.027
	O	0.410016
	Mg	0.002
	P	0.070
	S	0.002
	Ca	0.147
Lung	H	0.103
	C	0.105
	N	0.031
	O	0.749
	Na	0.002
	P	0.002
	S	0.003
	Cl	0.003
	K	0.002

Table 1

Proton beam and geometry parameters for comparing Geant4 to MCNPX simulations. In all SOBP simulations, the range was 17.2 cm and the modulation width was 5.0 cm.

Beam	Energy / MeV	Target	HBB
Monoenergetic	100	Water phantom	-
Monoenergetic	100	Water phantom	-
Monoenergetic	100	Water phantom	8 cm Lung
Monoenergetic	200	Water phantom	8 cm Lung
Monoenergetic	200	Water phantom	8 cm Bone
Monoenergetic	200	Water phantom	8 cm Bone
Monoenergetic	100	Complex phantom	-
Monoenergetic	200	Complex phantom	
SOBP		Complex phantom	-
SOBP		Water phantom	-
Monoenergetic	100	CT geometry	-