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The comparison of Monte Carlo simulations with GEANT4 for polyethylene absorber within the pCT development

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Proton beams in medical applications deal with relatively thick targets like the human head or trunk. Thus, the fidelity of proton computed tomography (pCT) simulations as a tool for proton therapy planning depends in general case on the accuracy of results obtained for the proton interaction with thick absorbers. As we previously showed it, the GEANT4 simulations of proton energy spectra after thick absorbers do not agree well with existing experimental data. Moreover, the spectra simulated for the Bethe-Bloch domain showed an unexpected sensitivity to the choice of low-energy electromagnetic models during the code execution. These observations were done with the GEANT4 version 8.2 during our previous simulations for pCT. As the most probable reasons for these effects is some specific feature in the code, or some specific implicit parameters in the GEANT4 manual, we continued our study with versions 9.2 and 9.4 of the code. This work describes in more details the simulations of the 25 MeV protons passing through 6mm polyethylene absorber. The simulations were done by modifying only the geometry in the Hadrontherapy Example, and for all available choices of the Electromagnetic Physics Models. The results were compared with our previous simulation, with theoretical predictions and with experimental data. Some variations in comparison with our previous results were obtained. The simulations were performed considering further applications for pCT development.

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1. Introduction

The interest in proton computed tomography (pCT) development is now reopened with the spread of the proton beam treatment [1]. The idea is to use the same medical proton therapy beam for diagnosis with pCT, i.e. for tumor localization and data acquisition for further irradiation planning. Potentially it can improve the quality of proton therapy and decrease the dose delivered to patients. The Monte Carlo simulations have a successful history in varied fields of study and could also be a helpful instrument in the case of pCT development.

Proton beams in medical applications deal with relatively thick targets like the human head or trunk. Thus, the fidelity of proton computed tomography (pCT) simulations as a tool for proton therapy planning depends in the general case on the accuracy of results obtained for the proton interaction with thick absorbers. As we previously showed it, the GEANT4 simulations of proton energy spectra after thick absorbers do not agree well with existing experimental data [2, 3, 4]. Moreover, the spectra simulated for the Bethe-Bloch domain showed an unexpected sensitivity to the choice of low-energy electromagnetic models during the code execution. These observations were done with the GEANT4 version 8.2 during our previous simulations. The most probable reasons for these effects is some specific feature in the code, or some specific implicit parameters in the GEANT4 manual. In this work we continued our study of the 25 MeV protons passing through 6mm polyethylene absorber with versions 9.2 and 9.4 of the GEANT4 code. The simulations were done by modifying only the geometry in the Hadrontherapy Example, and for all available choices of the Electromagnetic Physics Models. The results were compared with our previous simulation, with theoretical predictions and with experimental data.

2.Materials and Methods

2.1 Experimental Data

The experimental data used in this work as reference were taken from publication of Ito [5], where the spectrum of 25 MeV protons, after passing through 6.0 mm of 0.945 g/cm^3 polyethylene, was published. The spectrum was measured with a Si detector with 50 keV energy resolution (FWHM of the initial 25 MeV proton spectrum). All the main parameters of the experiment were published in detail except the distance between the detector and the outgoing accelerator foil, where the protons passed through air.

2.2 Energy Loss and Straggling Theory

When traversing matter, protons may be absorbed only in inelastic nuclear interactions. However, the total probability of these processes is small enough to be neglected when only the proton beam transport is under consideration. Thus, the Boltzmann kinetic equation for this case consists of only two integrals to describe the multiple Coulomb scattering on the nucleus and the electromagnetic interactions with atomic electrons [6].

There is no general analytical solution of the Boltzmann transport equation in this form. As the first integral describes the total effect of a large but finite number of interactions with the same nature, it is suitable to solve it via Monte Carlo simulations [7]. As the main contribution

of this term, a direction degradation of the initially parallel proton beam is assumed. Thus, it was called "elastic" integral [6]. The second integral is mainly responsible for the proton energy loss, and therefore has the name "inelastic" integral. Its calculation could be done analytically only within some significant simplifications [6], [7], [8]. In particular, within so-called "straight-forward" approximation the scattering of protons (i.e. the "elastic" integral) is totally neglected. The "inelastic" integral could be then expanded in series using the proton-to-electron energy transfer as a small parameter. The first term left of such expansion gives the Continuous Slowing-Down Approximation (CSDA) [6].

The CSDA is usually used to calculate directly the mean value of the final proton energy after passing through a layer of matter. It is also incorporated into Monte Carlo codes to calculate the mean energy loss between the elastic collisions [7], [9], [10], [11]. If we take into account one more term in the expansion of the inelastic collision integral, the transport equation will be transformed into the Fokker-Plank (diffuse) form [6]. For this case, Payne proposed the approximate self-consistent Gaussian solution [12]:

$$N(x,E)=\frac{N_0}{\bar{\omega}(E)}\times\frac{1}{\sqrt{2\pi\sigma^2(x)}}\exp\left[-\frac{\left(R_{CSDA}(E_{in})-R_{CSDA}(E)-x\right)^2}{2\sigma^2(x)}\right] \tag{1}$$

where

$$\sigma^2(x)=\left(\frac{m_e c^2}{4\pi r_e^2\eta}\right)^2\int_{E_{out}(x)}^{E_{in}}\frac{\left[\left(1+\frac{E}{m_p c^2}\right)^2-1\right]^3}{\left(1+\frac{E}{m_p c^2}\right)^4 F^3\left(\beta(E),I\right)}dE$$

Here E_{in} is the initial proton energy, $\beta(E)=v(E)/c$ is the proton velocity, m_p and m_e are correspondently the proton and the electron mass, r_e is the classical (Bohr) electron radius, η is the volumetric electron density, I is the averaged ionization potential

2.3 Statistical Analysis

In order to make a correct comparison of the spectra with different number of protons, all the spectra were reduced to the discrete Probability Density Functions (PDF) by using (2), where N_i is the number of protons in the i-th energy range – from E_i to $E_i+\delta E$, and N_0 is the total number of protons in the spectrum.

$$PDF_i=\frac{N_i}{N_0\cdot\delta E} \tag{2}$$

Consequently, the mean energies of protons in the spectra were calculated as (3).

$$\overline{E}=\delta E\sum_i\left(E_i+\tfrac{1}{2}\delta E\right)PDF_i \tag{3}$$

It should be noted that the spectra have a "tail" form, so that the mean energy does not exactly coincide with the most probable energy, i.e., the peak maximum position. The statistical errors were defined using the definition for standard deviation in the discrete case.

3. Monte Carlo Simulations

Some popular Monte Carlo packages could be used to study pCT development.

GEANT4 [13] is actually the most general framework for handling the motion of particles through matter. Its ability to work with very complex geometry and tracking is essential to the pCT development. The simulations were made with the versions 4.9.2 and 4.9.4 and compared with our previous results with 4.6 and 4.8.2 versions.

SRIM/TRIM is historically one of the first Monte Carlo codes for ion transportation, actually with the friendliest interface. In this work, we used the TRIM code from the SRIM 2011 version 6.0.

MCNPX is a general-purpose Monte Carlo radiation transport code developed at Los Alamos National Laboratory [14]. We were interested in this code because its applications include, among others, the proton therapy. The simulation was done using the MCNPX version 2.4.0.

4. Results and Conclusions

The Figure 1 shows the results of our previous and present simulations in comparison with the experimental data. The results of the statistical analysis of the spectra are shown in the Table 1.

It could be seen that the simulations under default execution mode have a trend to better approximate the experiment with the GEANT4 development, except for the 4.9.2 version. In addition, the simulations with the latest version 9.4 finally show the correct performance: there are no visible differences in the spectra from the Bethe-Bloch domain obtained with different models. Previously, starting from 8.2, and up to 9.2, our results were very sensitive for such manipulations. For example the GEANT4.8.2 execution with Ziegler2000 model leads to the drastic displacement of the spectrum to the higher energies. The newest versions of GEANT4 code have received some significant improvements in electromagnetic physics models [15]. Apparently, these changes are responsible for the better simulation results with the resent versions of the code. We are planning to continue this work involving other experimental data.

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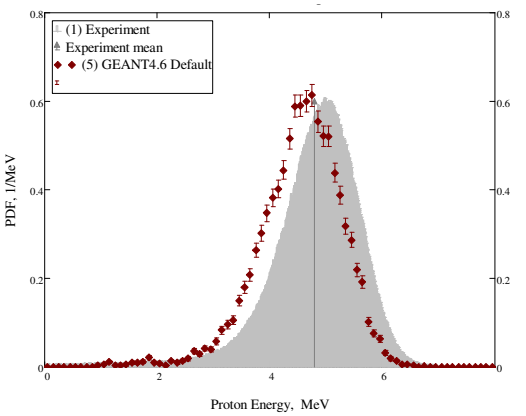
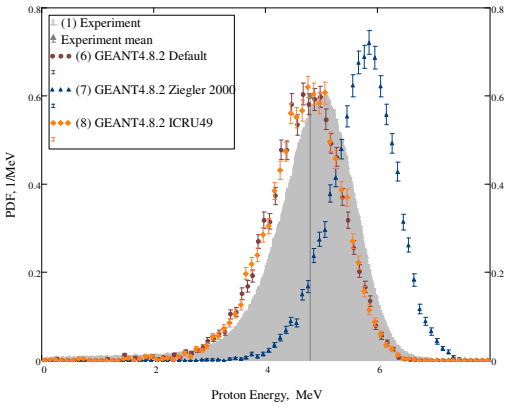
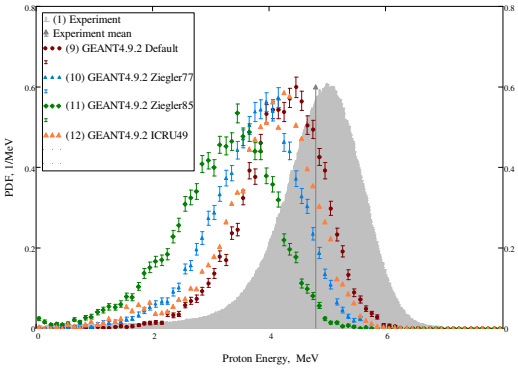


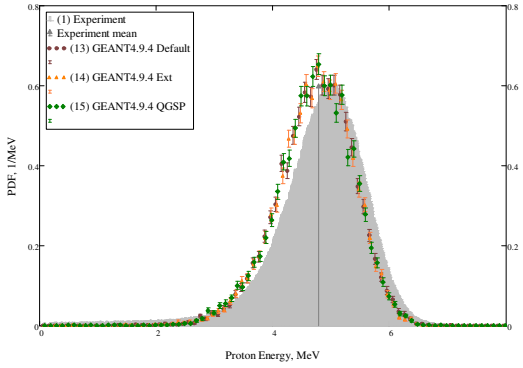
a) GEANT4.6



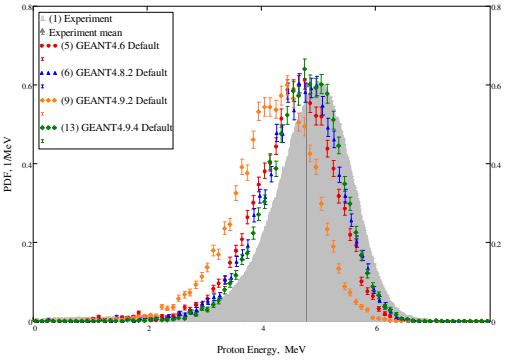
b) GEANT4.8.2



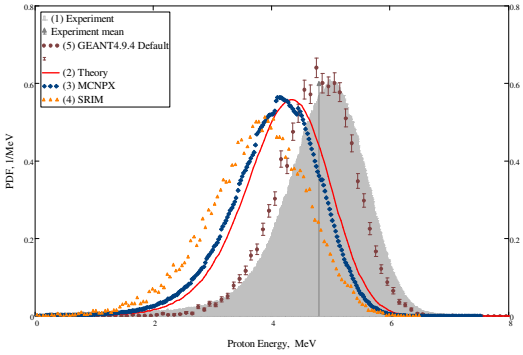
c) GEANT4.9.2



d) GEANT4.9.4



e) GEANT4 default models



f) GEANT4.9.4, Theory, MCNPX and SRIM

Figure 1- 25 MeV proton energy spectra after 6 mm polyethylene layer (simulated results and experimental data).

Table 1 - The mean energy and standard deviation for 6mm polyethylene layer

		<E>, MeV	σ, MeV
(1)	Experiment	4.791 ± 0.001	0.866 ± 0.001
(2)	Theory	4.186	0.751
(3)	MCNPX	4.045 ± 0.044	0.772 ± 0.031
(4)	SRIM/TRIM	3.602 ± 0.003	0.887 ± 0.002
(5)	GEANT4.6 Default	4.529 ± 0.007	0.745 ± 0.005
(6)	GEANT4.8.2 Default	4.653 ± 0.007	0.712 ± 0.005
(7)	GEANT4.8.2 Ziegler 2000	5.708 ± 0.006	0.603 ± 0.004
(8)	GEANT4.8.2 ICRU49	4.663 ± 0.007	0.702 ± 0.005
(9)	GEANT4.9.2 Default	4.189 ± 0.007	0.726 ± 0.005
(10)	GEANT4.9.2 Ziegler 77	3.720 ± 0.008	0.784 ± 0.006
(11)	GEANT4.9.2 Ziegler 85	3.184 ± 0.009	0.874 ± 0.006
(12)	GEANT4.9.2 ICRU49	3.924 ± 0.008	0.848 ± 0.006
(13)	GEANT4.9.4 Default	4.718 ± 0.007	0.662 ± 0.005
(14)	GEANT4.9.4 Extended	4.713 ± 0.007	0.665 ± 0.005
(15)	GEANT4.9.4 QGSP_BIC_EMY	4.712 ± 0.007	0.666 ± 0.005

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