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Evaluation of GATE/Geant4 multiple Coulomb scattering algorithms for a 160 MeV proton beam

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ABSTRACT

Purpose: To systematically evaluate simulated characteristic multiple Coulomb scattering (MCS) angles with GATE/Geant4 against experimental data for 158.6 MeV proton beams.
Methods: The open source toolkit GATE alongside Geant4 in release 9.5 patch 02, 9.6 patch 03, 10.0 patch 02, 10.1, and 10.2 patch 02 were used to simulate a 158.6 MeV collimated monoenergetic proton beam impinging on a scattering disc of various materials and thicknesses: in total 144 different set-ups were investigated per Geant4 release and compared to measured data. Data was read out into a phase space providing information of individual particle momentum. For analysis a one dimensional Gaussian was fit to the beam profile and the multiple Coulomb scattering angles were calculated using the ROOT toolkit.
Results: The agreement between simulated and experimental data was found to be dependent on the Geant4 release. On average an agreement of −1.1% with a standard deviation of 3.4% was reached with Geant4 release 10.2. Increased differences were found for very thick targets close to the particle range and for older Geant4 versions employing the previous electromagnetic model, Urban MCS.
Conclusion: Multiple Coulomb scattering algorithms implemented in the latest Geant4 releases and in particular Geant4.10.2 showed a very satisfactory agreement with measured data for applications in proton pencil beam scanning.

1. Introduction

Proton beam therapy is becoming more widely available, with more than 100 000 patients being treated so far [1]. Active beam scanning is a time-dependent method of achieving a desired dose distribution by magnetically moving the pencil beam across the target cross-section while dynamically changing the energy of the beam and, consequently, the depth of penetration.

To ensure accurate dose calculation, not only the range but also multiple Coulomb scattering interactions of every single pencil beam delivered must be precisely computed in the patient tissues. With increasing penetration depth, the characteristic multiple Coulomb scattering (MCS) angle increases, leading to broader transverse dose profiles.

The MCS theory developed by Moliere [2] describes the evolution of MCS angles in a homogeneous material. Its angular distribution consists of a Gaussian distribution for smaller angles, and a non-Gaussian tail contributing only about 1% of the total dose. On average, Moliere theory showed an accuracy within 1% [3].

General purpose MC codes are often used to benchmark various dose calculation algorithms and dedicated calculation codes and treatment planning systems used in particle beam therapy [4,5]. Therefore, a detailed comparison of MCS models in modern general purpose MC codes with reference measurements is of paramount importance.

While proton scattering algorithms have been evaluated in several papers [6,7] these studies mainly focused on the evaluation of transverse dose profiles. Differences between measured and simulated beam sizes through various PMMA thicknesses for a proton pencil beam at 230 MeV were up to 20% for the previous Geant4 release 9.2 [6]. Differences on transverse dose profiles calculated using the MC codes Geant4, PHITS and MCNP were reported of the order of 15% [6]. The study did not allow to determine which

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code is more accurate. One of the issues is that evaluating transverse dose profiles does not allow separating effects due to MCS from the beam transport algorithm.

In this paper, we focus on the evaluation of the simulated characteristic MCS angle, instead of the transverse dose profiles, in order to decouple differences due to MCS algorithms and differences due to the transport algorithm.

2. Materials and methods

2.1. Reference data

The extensive experimental data set from Gottschalk et al. [3] was selected for benchmarking purposes in our study. Over a period of more than 20 years MCS angles were measured at the Harvard Cyclotron Laboratory. All simulation results will be compared to this measured data set. In this manuscript difference is always referred to as simulation result minus the reference value. As the details of the experiment can be found in literature [3], only a short summary is given here. A 158.6 MeV proton beam, collimated to an initial sigma of 2 mm, impinged on a scattering disc. 14 materials, including high and low z materials (beryllium, polystyrene, carbon, lexan, nylon, lucite, Teflon, aluminium, copper, zinc, brass, tin, lead, uranium) were measured covering a wide range of normalized target thicknesses, defined as the target thickness divided by the particles range [3], varying from 0.002 to 1.02. At $z_2 = 100$ cm downstream of the scattering disc the beam profile was measured using a diode (see Fig. 1). Each position x_i of the beam profile, was converted to angles θ_i by using

$$\theta_i = \arctan\left(\frac{x_i}{z_E}\right). \quad (1)$$

The effective scattering distance z_E was determined by measuring the beam width at two positions sufficiently downstream to achieve an asymptotic behaviour (z_1 and z_2) and geometrical calculation [3].

The resulting Gaussian shaped distribution was fitted using a least square minimization. Non Gaussian contributions were too small to be measured in the experimental set-up and therefore omitted.

2.2. Simulation set-up

The simulation set-up was designed in close correspondence to the experimental set-up by Gottschalk et al. [3] as described above.

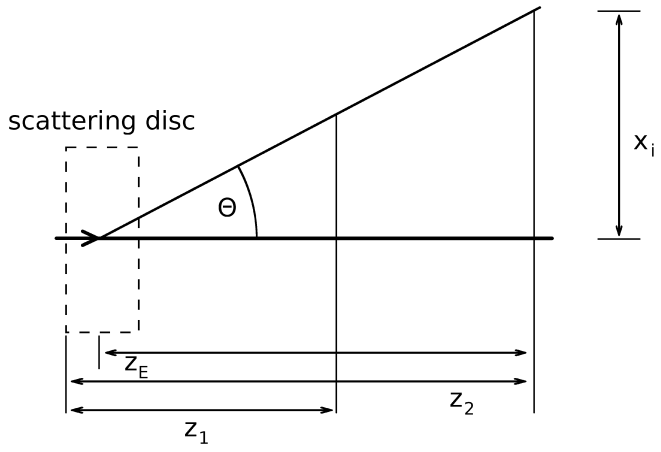

Fig. 1. Experimental set-up reproduced in simulation [3]. Indicated is the effective scattering distance z_E used for the experimental data, as well as $z_1 = 50$ cm and $z_2 = 100$ cm marking the position of the dose read out for back projection.

A 158.6 MeV proton beam with an initial sigma of 2 mm, having zero beam divergence impinged on scattering discs of the same materials and thickness as above (see Fig. 1). In total 144 different simulation set-ups with 10^7 protons each were created for each Geant4 release. For easier reference a list of materials used and their composition is given in the Appendix A in Table 3 [3].

The directional information of each particle was recorded after the scattering disc and stored in a phase space. Additional dose read outs were located 50 and 100 cm after the scattering disc, recording two dimensional beam profiles in order to enable a back projection of the beam width to determine the MCS angles. Particle propagation after the scattering disc was performed in vacuum to facilitate the comparison.

2.3. GATE/Geant4 simulation environment

GATE (Geant4 Application for Tomographic Emission) is an open-source software developed by the OpenGATE collaboration [8,9] dedicated to Monte Carlo (MC) simulations in medical physics.

Being a Geant4 application, it relies on the physics models of Geant4 [10,11], making it an ideal candidate to test the underlying physics models. Data analysis was performed using the data analysis framework ROOT [12] in version 5.34.

2.4. Physics models and parameters in Geant4

Generally, two models are used in Geant4 for proton MCS. The Urban MCS model, based on Lewis theory [13–15], was the default Geant4 MCS model until Geant4 version 10.1. For electrons this model is known to provide varying simulation accuracy depending on the selected step size and particle production limits. Similarly it was shown that step size has an influence on the MCS of protons [16]. The second model is the newer WentzelVI, employing the Wentzel MCS scattering function [17,18] for small scattering angles below 0.2 radian, while higher scattering angles are calculated using the single Coulomb scattering model, used in Geant4 version 10.2.

In Geant4 physics processes are implemented using different models. The user has to compile his own collection of physics processes and parameters. In newer versions of Geant4 this is facilitated by pre-defined physics lists, which are created by so called physics lists builders. Various electromagnetic (EM) physics model parametrizations are available within Geant4, option 0 to option 4. Using the new physics list builders, these can distinguished by the suffix EMV, EMX, EMY and EMZ for option 1–4, while no suffix indicates the use of the default, option 0. In Table 1 an overview is given of the main EM parameters for protons. For protons, option 0–2 are the same with respect to MCS. Option 3 and 4 employ the same MCS model. An evaluation of MCS angles simulated with all EM options was performed and indicated an influence of the selected MCS model (WentzelVI or Urban) on the simulated MCS

Table 1
Geant4 EM physics models and parameters used for protons in Geant4 release 10.2.

EM option	option 0–2	option 3	option 4
MCS physics model	WentzelVI	UrbanMCS	WentzelVI UrbanMCS until release 10.1
Binning (bins/decade)	7 bins	20 bins	20 bins
Stepping Algorithm	Minimal	Minimal	Minimal
Ionisation step limit finalRange	0.2	0.2	0.1
Ionisation step limit dRoverRange	0.1 mm	0.05 mm	0.02 mm

angles. The impact of the other parameters (see Table 1) was found to be negligible.

As was shown before in [6], Binning, step limits, and the choice of nuclear elastic and inelastic models influence the physical dose distribution. The Geant4 electromagnetic working group recommends option 4 [19] for all applications requiring high accuracy. Large angle scattering due to nuclear interactions might be influenced by the choice of nuclear models, but this contribution was reported to be in the off axis tail, contributing less than 1% [3].

Therefore, all further simulations were performed using QBBC_EMZ for Geant4 releases 9.6 patch 03, 10.0 patch 02, 10.1, and 10.2 patch 02 alongside GATE version 7, 7.1, and 7.2. Geant4 release 9.5 patch 02 alongside GATE version 6.2 was tested using the physics lists recommended in [6]. In order to compare only differences due to the MCS model, previously recommended simulation parameters for proton pencil beam scanning [6] were applied on top of the physics list. Finally, an additional configuration of Geant4 release 10.1 alongside Gate 7.1, using the physics list QBBC and a modified EM option 4 with WentzelVI instead of UrbanMCS was investigated.

2.5. Direct MCS angle evaluation

The scattering angle Θ describes the standard deviation of the Gaussian shaped angular distribution of a beam after scattering in a media. Direction vectors, normalized to a length of unit, extracted from the phase space files were converted to scattering angles Θ_i of the individual particles i by using trigonometric functions.

The resulting Gaussian shaped scattering angle distribution were fitted using the least square minimization routine MINUIT of the ROOT framework. Data points of less than 10% of the maximum were not considered for fitting, excluding low statistics noise, contributions of large single angle scattering and nuclear contributions.

2.6. Back projection of dose profiles

MCS angle was also determined using a second method, by mimicking the analysis of the measured transverse profiles as in [3]. Using two dose read outs sufficiently downstream of the scattering disc, two dimensional dose profiles were taken. At each position z_1 and z_2 downstream of the scattering disc, the beam width was determined using a Gaussian fit using the same method as before. Using the beam width at the two positions z_1 and z_2, the MCS angle was determined by back projection (see Fig. 1).

3. Results and discussion

For very thick targets close or even beyond the particle range, agreement of simulation results to the experimental data was worst, showing deviations of more than 10%.

The accuracy of the measurements and MCS theory in this region is questionable [3].

As these differences most likely are not caused by the modeling of multiple Coulomb scattering, we have restricted our analysis to material thicknesses below our MC particle range evaluated at 80% of the distal dose fall-off. For the sake of completeness all data points are included in the graphical representations.

A summary of the evaluations is provided in Table 2. A graphical representation of the differences between measured and simulated values for the Geant4 release 10.1 can be found in Fig. 2 for a selection of 6 materials. A more detailed figure containing all simulated data can be found in the Appendix A (see Fig. 4). There are two approaches for evaluation: averaging differences over all data points from all materials or taking the average of the average differences calculated per material, yielding slightly different results. In this paper the second method was considered. For Geant4 release 10.2 differences ranging from −17.8% to 10.9% compared to measurement data were evaluated, with an average difference of −1.1%, and a standard deviation of 3.4%.

Table 2
Difference of MCS angles determined using a one dimensional Gaussian fit of the individual Proton scattering angles, compared to reference data [3]. Values given are averaged over measurement points or per material, and normalized to reference data.

Geant4 release	diff ± SD [%] avg. per material	diff ± SD [%] avg. all points	range [%] for all points
9.5 p02	-9.7 ± 7.3	-9.3 ± 8.4	[−24.9; 13.1]
9.6 p03	-4.8 ± 3.5	-4.0 ± 4.8	[−23.0; 8.9]
10.0 p02	-5.2 ± 4.9	-4.7 ± 5.6	[−23.0; 8.3]
10.1	-5.2 ± 4.8	-4.8 ± 5.5	[−22.7; 8.1]
10.1 opt 4 Wentzel	-1.2 ± 3.3	-0.7 ± 4.8	[−17.9; 11.2]
10.2	-1.1 ± 3.4	-0.6 ± 4.9	[−17.8; 10.9]

Most of the materials tested showed slightly lower scattering than expected from experiment. Simulated MCS angles for very high z materials like brass, lead and uranium gave higher values using MC compared to measurements. This corresponds with the observation of Gottschalk [3] that MCS theory resulted in too high values for very thick targets consisting of higher z materials.

Agreement between simulation and measured data points were found to be dependent on the Geant4 release. Overall, the deviations to measurements reduces with newer Geant4 releases. Statistical variance of the scattering angles of individual particles was limited by the high number of simulated particles. The employed fitting process is resistant to noise, with residuals typically below 1^{-3} mrad, which is far below the measurement uncertainty.

An additional electromagnetic model, WentzelVI, was introduced into Geant4 in 2010 [20]. In Geant4 version 10.1 it was already used for protons in EM option 0–2, showing slightly larger MCS angles compared to the UrbanMCS model in use in EM option 3–4. Starting with Geant4 version 10.2 WentzelVI is now used in all EM options (0–4). The data showed a significant improvement in accuracy compared to older versions. To ensure this was caused by the model change and not some other code optimization, the Geant4 EM option 4 physics builder source code of version 10.1 was modified to use the WentzelVI model. As can be seen in Table 2 the results agree very well with the newer Geant4 release. All values were shifted towards the reference data, conserving the earlier

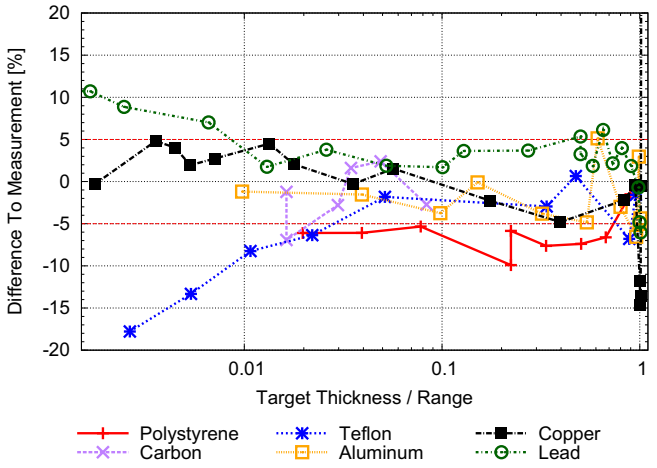

Fig. 2. Differences between measured [3] and simulated MCS angles, normalized to the measured data for a selection of 6 representative materials. Simulated using GATE v7.2 and Geant4 release 10.2 with EM option 4 (WentzelVI MCS). The lines connect the simulated data points and are drawn to guide the eye.

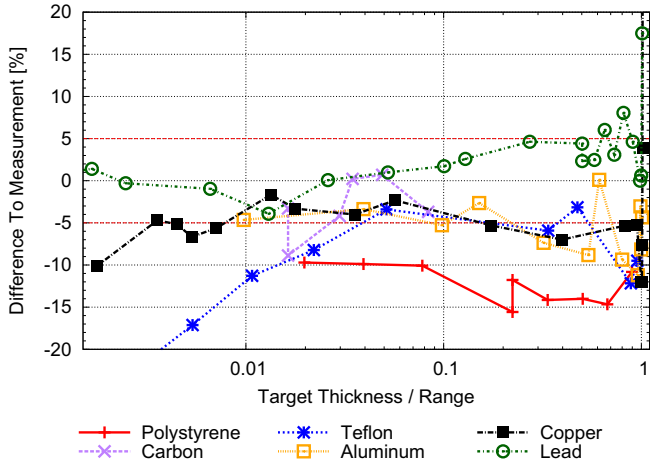

Fig. 3. Differences between measured [3] and simulated MCS angles, normalized to the measured data for a selection of 6 representative materials. Simulated using GATE v7.1 and Geant4 release 10.1 with the previous EM option 4 (Urban MCS). The lines connect the simulated data points and are drawn to guide the eye.

curve shapes with UrbanMCS model (see Fig. 3). For Geant4 release 10.1 with the custom added WentzelVI model, differences ranging from −17.9% to 11.2% compared to measurement data were evaluated, with an average difference of −1.2%, and a standard deviation of 3.3%.

Even though EM option parameters were kept the same between releases, the MCS angles changed, indicating that the underlying physics model implementations and data sets or some internal parameters were different.

Back projection of dose profiles, mimicking the evaluation of the measurement data, were performed as a consistency check. For Geant4 release 10.1 back projection resulted in an average difference of −4.3%, a standard deviation of 6.4% distributed from −21.7% to 9.4% compared to measurement data. Higher deviations were found for very small as well as very big MCS angles as occurring for high z materials with thicknesses close to the particles range.

A comparison with the direct phase space evaluation method indicated no adverse influences, as both methods (with and without transport algorithm) are in satisfactory agreement. Furthermore, a comparison of both methods served as a consistency check for the analysis.

The wide range of materials investigated allows a good overview of the overall effectiveness of MCS models. Some of the investigated materials, such as uranium, are less relevant in clinical practice. However, among others, materials such as copper, aluminum, or Teflon are likely to be present in beam line monitors and vacuum windows. Due to their distance from the iso-center even small amounts of scattering material will have a significant impact on beam width and needs to be carefully modelled.

Recently, MCS angles from theoretical predictions were compared with Geant4 simulations of a single release [21]. Makarova et al. described a slight underestimation of MCS angles for low-Z targets, while high-Z targets were overestimated, which agrees well with our results. Their data shows an agreement from low to high-Z targets of −8% to 1% for the UrbanMSC and −4% to 5% for the newer WentzelVI MSC model, a behaviour which can be also be seen in Fig. 3 and 2 above. Overall, their reported deviations are smaller, due to the comparison with theoretical models than with experimental data, but their findings show the same agreement and behaviour as shown above.

4. Summary and conclusion

A systematic comparison of MCS angles determined using GATE/Geant4 based Monte Carlo simulations with experimental data was performed. Overall, a good agreement with measured data for applications in proton pencil beam scanning was found. The newly implemented WentzelVI MCS model caused a significant improvement in MCS angle accuracy. Simulated MCS angles were slightly below the experimental values, on average agreeing within −1.1% of measurement values, with a standard deviation of 3.4% with Geant4 release 10.2. Increased differences were found for very thick targets close to the particle range.

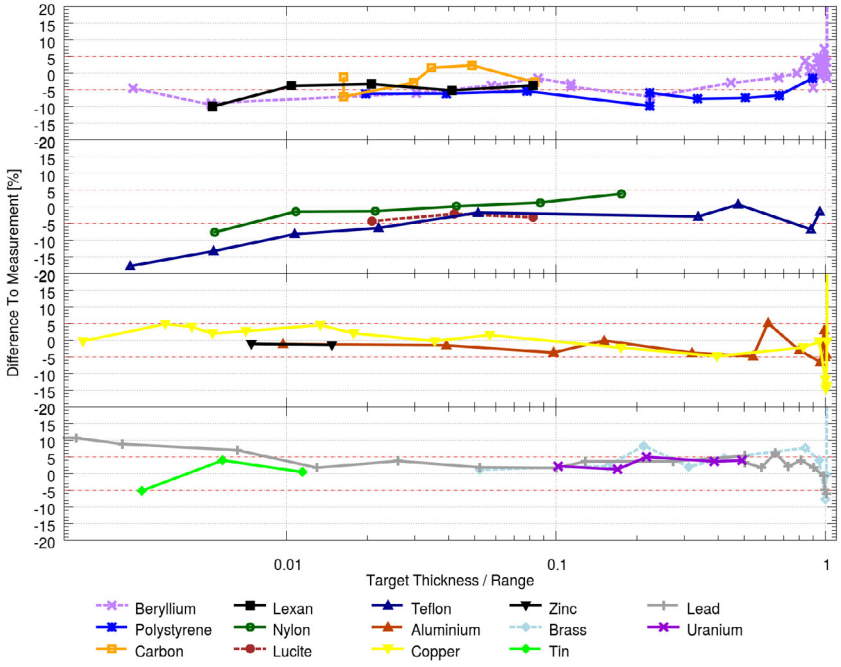

Fig. 4. Differences between measured [3] and simulated scattering angles, normalized to the measured data for all materials. Simulated using GATE v7.2 and Geant4 release 10.2 with EM option 4 (WentzelVI MCS). The lines connect the simulated data points and are drawn to guide the eye.

Table 3
Physical and chemical composition of materials used.

Material	Fractional weight	Z	A [g/mol]	Density [g/cm^3]	Range [g/cm^2]
Beryllium		4	9.012	1.853	21.1781
Polystyrene				1.032	17.5680
C	0.923	6	12.011		
H	0.077	1	1.008		
Carbon		6	12.011	2.220	19.3424
Lexan				1.200	17.6850
C	0.741	6	12.011		
O	0.185	8	15.999		
H	0.074	1	1.008		
Nylon				1.130	17.1596
C	0.549	6	12.011		
O	0.244	8	15.999		
N	0.107	7	14.007		
H	0.100	1	1.008		
Lucite				1.200	17.5624
C	0.600	6	12.011		
O	0.320	8	15.999		
H	0.081	1	1.008		
Air				0.001	
N	0.745	7	14.007		
O	0.229	8	15.999		
Ar	0.026	18	39.948		
Teflon				2.200	20.8622
F	0.760	9	18.998		
C	0.240	6	12.011		
Aluminum		13	26.981	2.700	22.1543
Copper		29	63.540	8.960	
Zinc		30	65.370	7.133	
Brass				8.489	25.7386
Cu	0.615	29	63.540		
Zn	0.352	30	65.370		
Pb	0.033	82	207.190		
Tin		50	118.690	7.298	30.0524
Lead		82	207.190	11.350	34.8831
Uranium		92	238.030	18.700	35.5468

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Appendix A

(see Fig. 4).

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