

Fast SDE-based Monte Carlo dose calculation for proton therapy validated against Geant4

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Abstract

Objective: To validate a newly proposed stochastic differential equation (SDE)-based model for proton beam energy deposition by comparing its predictions with those from Geant4 in simplified phantom scenarios.

Approach: Building on previous work in Crossley et al. (2025), where energy deposition from a proton beam was modelled using an SDE framework, we implemented the model with standard approximations to interaction cross sections and mean excitation energies, which makes simulations easily adaptable to new materials and configurations. The model was benchmarked against Geant4 in homogeneous and heterogeneous phantoms.

Main results: The SDE-based dose distributions agreed well with Geant4, showing range differences within 0.4 mm and 3D gamma pass rates exceeding 98% under 3%/2 mm criteria with a 1% dose threshold. The model achieved a computational speed-up of approximately fivefold relative to Geant4, consistent across different Geant4 physics lists.

Significance: These results demonstrate that the SDE approach can reproduce accuracy comparable to high-fidelity Monte Carlo for proton therapy at a fraction of the computational cost, highlighting its potential for accelerating dose calculations and treatment planning.

Keywords: Monte Carlo simulation, proton therapy, radiation transport modelling, jump stochastic differential equation, dose calculation

1 Introduction

Accurate dose calculations are critical for proton therapy treatment planning to ensure precise treatment delivery while minimising uncertainties in patient outcomes. Thus, high-fidelity models are needed to capture the inherently stochastic nature of proton interactions in tissue, including energy loss, scattering, and nuclear interactions. Currently, pencil beam algorithms (Hong et al. 1996, Schaffner et al. 1999) are the standard dose calculation technique in the clinical setting because of their computational efficiency, which allows for fast treatment planning. However, they achieve speed at the expense of accuracy. Pencil beam algorithms perform reliably in homogeneous media and provide good agreement for depth-dose profiles, but struggle to accurately model lateral spread, tissue heterogeneities, and complex geometries. Due to this, Monte Carlo (MC) models such as Geant4 (Agostinelli et al. 2003), TOPAS (Perl et al. 2012), GATE (Grevillot et al. 2020) and FLUKA (Böhlen et al. 2014), among others, are an alternative to analytical methods to perform the most accurate dose calculations, which can reduce the error margins by several millimetres (Paganetti 2012). This is achieved by tracking each proton step by step and sampling each possible interaction according to its probability, which means this method tends to be much slower, compromising computational efficiency and therefore its suitability for routine treatment planning.

GPU-based implementations such as MOQUI (Lee et al. 2022) enable highly efficient dose scoring, while other approaches avoid simulating secondary particles to fully exploit GPU computing power (Shan et al. 2022). On the CPU side, optimised codes such as MCsquare (Deng et al. 2020) leverage multi-core architectures to achieve substantial reductions in computation time. These developments are bringing MC closer to routine use in treatment planning and plan verification. However, achieving near real-time performance for adaptive therapy or robust optimisation remains challenging, particularly for complex patient geometries and medical images with a large number of voxels.

To address this gap, new mathematical approaches are needed for modelling proton beam treatment delivery, aiming to lie between high-fidelity Monte Carlo accuracy and pencil beam algorithm efficiency. Ashby et al. (2024) proposed an approach based on optimisation by computing the fluence of the associated Boltzmann transport equation numerically. In Crossley et al. (2025), a complementary approach was introduced to solve the Boltzmann transport equation in backward form using a jump stochastic differential equation (SDE). The latter retains the probabilistic nature of Monte Carlo simulations while replacing frequent small-angle Coulomb scatterings with a physics-informed diffusion term. This reduces computational cost without sacrificing physical fidelity due to the central limit theorem. Moreover, Kyprianou et al. (2025) showed that the two methods are consistent in the sense that they are alternative but compatible mathematical descriptions of the same underlying dynamics, expressed in terms of macroscopic fluence on the one hand and microscopic particles on the other. The reduced runtime of the proposed SDE approach compared to full Monte Carlo simulations makes it an attractive candidate for tasks such as plan verification, robustness evaluation, and adaptive planning, where high accuracy is required but computational cost remains a limiting factor.

In this article, we present an enhanced version of the SDE model with cross sections designed to match physical quantities. We compare its predictions to Geant4 as a reference standard using homogeneous and heterogeneous phantoms, and quantify both accuracy and

computational speed. The two main objectives of this work are:

- To show SDE-based methods provide accurate dose predictions at low computational cost in clinically relevant settings when compared to current Monte Carlo codes.
- To highlight the inherent adaptability of the SDE framework, capable of accommodating a broad spectrum of model complexities, thus establishing a foundation for future optimisation based on clinical need.

2 Microscopic proton physics

The fundamental basis of proton beam therapy is the principle of high energy protons decelerating through their interactions with subatomic particles in the surrounding tissue. Deceleration is synonymous with energy deposition, and this energy transfer is a key component of attacking cancerous tissues.

As the energy of a proton decreases, its rate of interaction with subatomic particles increases, leading to a greater rate of energy deposition. This means that, to a certain extent, the location at which the majority of the energy from a proton beam is deposited is controllable, causing minimal exposure to surrounding healthy tissues. Indeed, the energy deposition can be arranged in a way that there is no exit dose from a proton beam directed towards tumour tissues. These particular phenomena distinguish proton beam therapy from photon therapy.

In Crossley et al. (2025), the basic principles of atomic physics were used to build a mathematical model for the dynamics of protons in a proton beam travelling through matter in three-dimensional space. The principal mathematical tool was a so-called stochastic differential equation (SDE) with jumps. The SDE method lends itself well to new Monte Carlo approaches which favourably balance accuracy and computational cost.

We begin with a brief reminder of the physics of proton beams and how this plays into the modelling choices that lead to the SDE formulation, which is introduced in the subsequent section. For a more detailed read on the background physics of proton beams, the reader is referred to Newhauser & Zhang (2015), Paganetti (2020) and Gottschalk (2018), among many possible sources.

2.1 Proton interactions

In order to describe the evolution of protons, we need to introduce the space-direction-energy phase space in which they live. To that end, let $D \subset \mathbb{R}^3$ denote a closed and bounded convex spatial domain, \mathbb{S}_2 be the unit sphere in \mathbb{R}^3 and $\mathcal{E} = [e_{\min}, e_{\max}] \subset [0, \infty)$ be the range of energies a proton can take. We thus define the energy-position-direction phase space as $\mathcal{C} = \mathcal{E} \times D \times \mathbb{S}_2$.

Consider now a proton travelling through matter with an instantaneous configuration $x = (\epsilon, r, \omega) \in \mathcal{C}$. In order to describe the dynamics of an individual proton, we consider the notion of transport and three broad types of atomic interactions with surrounding matter (See Figure 1). We refer the reader to Newhauser & Zhang (2015) for further details. These mechanisms are:

Transport. In the space between atoms, the proton moves in straight lines in the direction ω .

Inelastic Coulomb interaction. We assume that protons lose energy continuously as a consequence of a large number of collisions with orbital electrons. For an instantaneous configuration $x = (\epsilon, r, \omega)$, there are two contributing factors to this continuous energy loss. Deterministic loss which occurs at a rate (per unit track length) given by what is commonly referred to as the *stopping cross section*, $\varsigma_1(x)$. We model variability in the number of orbital electron collisions per unit track length by an additional stochastic loss term, governed by a Brownian motion whose volatility is given by what is commonly referred to as the *energy-straggling cross section* $\varsigma_2(x)$. We assume that these collisions have no effect on the direction of motion of the relatively massive proton, or equivalently, that any effect is subsumed into the elastic scatter term described below.

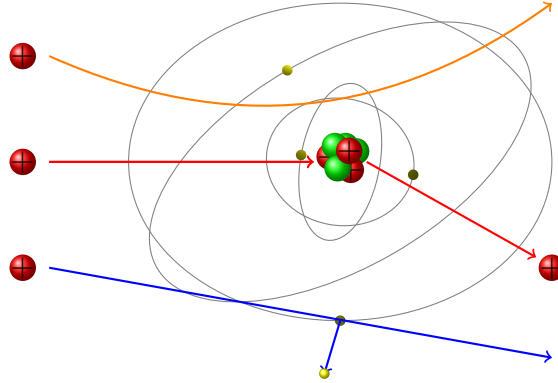


Figure 1: The three main interactions of a proton with matter. An elastic scattering (top) with the nucleus, a proton-nucleus collision which may be elastic or inelastic (centre), and an inelastic Coulomb interaction with atomic electrons (bottom).

Elastic scatter. This class of events corresponds to a change in direction of the proton due to an interaction with a nearby nucleus whilst conserving energy between the proton and the nucleus. The three types of elastic scattering events we consider are as follows:

Elastic Coulomb scatter: The proton passes sufficiently close to an atomic nucleus that it feels a repulsive positive charge, resulting in a change in its direction of motion. We distinguish between two cases: large and small scatters. For incoming direction ω and outgoing direction ω' , let $\theta \in [0, \pi]$ denote the polar scattering angle. Then, we fix a small cut-off, say $\delta > 0$, such that the case $\theta > \delta$ is termed a large (elastic Coulomb) scatter and the case $\theta \leq \delta$ is called a small scatter. We use a cross section $\sigma_e(x)\pi_e(x; d\omega')$ to mathematically describe large scatter events, where $\sigma_e(x)$ denotes the rate at which a proton with configuration $x = (\epsilon, r, \omega) \in \mathcal{C}$ undergoes a large elastic Coulomb scatter, and the probability density $\pi_e(x; d\omega')$ describes the distribution of the resulting outgoing direction ω' . Small scatter events are subsumed into an aggregated term, described below. In the (medical) physics literature, it is not uncommon to think of $\sigma_e(x)$ as a rate per unit track length, which captures the amount of atomic interactions a proton has with the medium through which it travels.

Elastic proton-nucleus collision and scatter: In rare cases, the incoming proton is absorbed into the nucleus, which then becomes excited, resulting in a proton being released with the same energy as the incoming proton. Since protons are indistinguishable, we model them

identically to the elastic Coulomb scatters described above, so that σ_e and π_e are the cross section and probability density of both event types combined.

Coulomb-nuclear interference: It is insufficient to treat both the effects of elastic Coulomb scattering and elastic proton-nucleus collisions independently (Nekrasov 2024). The combination of these effects results in an additional perturbation in the outgoing angle due to so-called Coulomb-nuclear interference. We take the same cut-off δ to distinguish between small and large scatters, where large scatters are subsumed into the elastic Coulomb scatter and small scatters subsumed into the aggregation of small scatter, described below. Mathematically, σ_e and π_e incorporate Coulomb-nuclear interference as well.

Aggregated small scatter. We consider the net effect of all small scatter events to result in a diffusive component in the direction of motion ω of protons (Vassiliev 2017, Section 3.9.6). More precisely, the direction of transport ω undergoes a state-dependent Brownian motion on \mathbb{S}_2 with volatility $m(x) \geq 0$ where x is the instantaneous configuration of the proton. As with large scatter events, we assume there is no energy loss associated with these small scattering events.

Inelastic proton-nucleus collision and scatter. When a proton interacts with a nucleus, it can undergo an inelastic collision, forming an excited nuclear state. This excited nucleus may subsequently emit a spray of secondary particles, transferring some of its energy to each particle. For the SDE model considered in this article, we assume that each collision will emit exactly one secondary proton which carries the majority of the outgoing energy and outgoing direction ω' . The energy deficit between the incoming and outgoing protons is accounted for by the recoil of the nucleus, other secondary particle emission which our SDE neglects, and the binding energy of the interaction.

As will be made evident in Section 6, even with this secondary particle simplification, the accuracy of our model performs well against current Monte-Carlo codes without invoking the computational overhead incurred by these additional secondary tracks. Moreover, we emphasise that the SDE framework allows for multiple secondary particles, thus facilitating a hierarchical collection of models that trade computational cost for further accuracy. The result of this extension is a branching SDE, where SDEs of the form (1) are fitted to each particle type. However, for the scope of this article, we focus on how to fit a single type SDE for protons and leave this extension for future research.

Nuclear inelastic scatters occur according to the cross section $\sigma_{ne}(x)$, seen as a rate per unit track length, in which case the configuration, x , of the incoming proton is transferred to an outgoing configuration $x' = (\epsilon(1 - u), r, \omega')$ with probability density $\pi_{ne}(x; d\omega', du)$, where $u \in (0, 1]$.

2.2 Sequential proton tracks

In Crossley et al. (2025), the notion of a *sequential proton track* was introduced to describe the evolution in configuration-space of an initial proton concatenated with subsequent protons that continue its trajectory after proton-nuclear interactions, ultimately to absorption or a de-energised state. The terminus point of the sequential proton track is called its *range*. Each sequential proton track is a random trajectory and we can think of a *proton beam* as being made up of many superimposed sequential proton tracks. Without loss of generality,

it is assumed that each sequential proton track behaves independently and therefore, up to a scaling factor, by the Law of Large Numbers, the proton beam is nothing more than the average effect of an individual sequential proton track.

2.3 Bragg peak

The Bragg peak is a graphical representation of the energy deposition per unit length along the axial direction of a proton beam. A typical Bragg peak curve is proportional to the average energy deposition per unit length along sequential proton tracks. Its characteristic shape, illustrated in Figure 2, shows a gradual increase in energy deposition followed by a sharp rise near the end of the proton range, and then a rapid fall-off. One of the defining features of the Bragg peak is its range, defined as the depth at which the dose falls to a predefined fraction of its maximum. Quantities such as R90 and R50, defined as the depths at which the dose falls to 90% and 50% of the maximum, respectively, are commonly used in the literature.

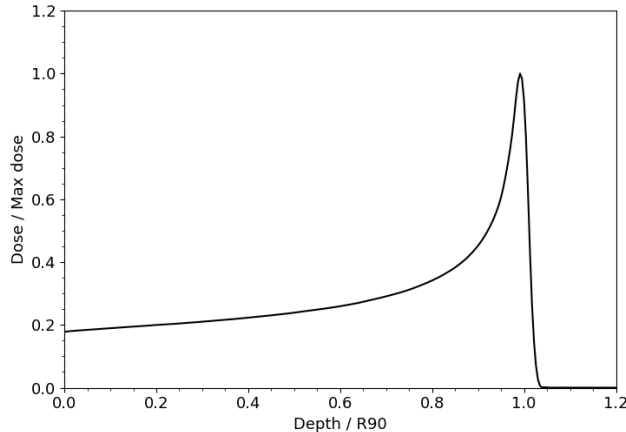


Figure 2: A typical Bragg Peak curve in a homogeneous medium. Depth is normalised to the proton range R90, and dose is normalised to its maximum value.

3 Sequential proton track SDE

To model the evolution of a proton’s trajectory through the configuration space \mathcal{C} , we employ an enhanced version of the SDE first introduced in Crossley et al. (2025). We follow the vast majority of physics and nuclear literature, and index our SDE by the inherent ‘track length’ of the sequential proton track that it describes. We define the dynamic evolution of the configuration variables along a sequential proton track via $(Y_\ell, \ell \geq 0) = ((\epsilon_\ell, r_\ell, \omega_\ell), \ell \geq 0)$, where ϵ_ℓ is the energy at track length $\ell \in \mathcal{E}$ of the sequential proton track, $r_\ell \in D$ is the position of the sequential proton track at track length ℓ , and $\omega_\ell \in \mathbb{S}_2$ is its direction of transport. The process Y represents the random evolution of a sequential proton track in configuration space \mathcal{C} .

Since our focus is on simulating the sequential proton track, we introduce the evolution of Y in terms of its Euler—Maruyama approximation, a standard numerical scheme for

approximately simulating SDE paths. We will work on the lattice track lengths ($\ell = \Delta n, n \geq 0$), where $\Delta > 0$ is a small increment of path length. The collective evolution of $Y_n := (E_n, R_n, \Omega_n) := (\epsilon_{\Delta n}, r_{\Delta n}, \Omega_{\Delta n})$, for $n = 0, 1, 2, \dots$ is governed by

$$\boxed{\begin{aligned} E_{n+1} &= (E_n - \varsigma_1(Y_n)\Delta + \min\{\max\{\varsigma_2(Y_n)B_n, -\varsigma_1(Y_n)\Delta\}, \varsigma_1(Y_n)\Delta\})(1 - u_n) \\ R_{n+1} &= R_n + \Omega_n\Delta \\ \Omega_{n+1} &= \Omega_n + m(Y_n)\Xi_n + D_n \end{aligned}} \quad (1)$$

where:

- B_n in an increment of Brownian motion with variance Δ and the corresponding random term on the right-hand side has been truncated to ensure non-increasing energy while preserving the correct continuous energy loss.
- Ξ_n is the time- Δ increment of spherical Brownian motion on \mathbb{S}_2 , simulated via Algorithm 1 of Mijatović et al. (2020). It models the aggregate effect of small scattering events on the direction of the proton.
- (u_n, D_n) takes value $(0, (0, 0, 0))$ with probability $1 - e^{-\Delta(\sigma_{ne}(Y_n) + \sigma_e(Y_n))}$, and otherwise is sampled from the mixture distribution

$$\begin{aligned} \pi(Y_n; d\Omega', du) &:= \frac{\sigma_e(Y_n)}{\sigma_e(Y_n) + \sigma_{ne}(Y_n)} \pi_e(Y_n; d\Omega') \delta_0(du) \\ &\quad + \frac{\sigma_{ne}(Y_n)}{\sigma_e(Y_n) + \sigma_{ne}(Y_n)} \pi_{ne}(Y_n; d\Omega', du). \end{aligned} \quad (2)$$

The former case corresponds to the absence of a large scattering event in the track length increment, while the latter corresponds to either an elastic ($u_n = 0$) or inelastic ($u_n \in (0, 1]$) scattering event.

The evolution in (1) continues until the proton exits the domain D , or its energy falls below the minimum threshold e_{\min} .

In the next section, we present our choices for the functionals $\sigma_e, \pi_e, \sigma_{ne}, \pi_{ne}, \varsigma_1, \varsigma_2$, and m . All are informed by the physics literature so that Y replicates the behaviour of a sequential proton track. This makes it possible to apply the SDE model to new materials simply by entering their chemical composition, mean excitation energy, and estimates of the nuclear scattering cross sections in ENDF format without the need to calibrate any free parameters.

4 Choices of SDE parameters

In this section, we describe our choices of parameters for the SDE introduced in Section 3. We will use well-established physics-based models or, when such models are not available, numerical approximations fitted to experimental nuclear data.

4.1 Inelastic Coulomb scattering

We recall from Section 3 that energy losses due to inelastic Coulomb interactions are incorporated into the SDE (1) through a deterministic rate given by ς_1 and stochastic fluctuations with volatility given by ς_2 . To justify this model choice, we give a brief exposition on the theory of inelastic interactions (see Salvat (2022) for further details). First consider the setting of a proton with configuration $x = (E, R, \Omega) \in \mathcal{C}$ travelling through a homogeneous medium consisting of a unique element. Each inelastic interaction involves a certain energy transfer $W \in [0, E]$ from the proton to the electrons of an atom in the medium. This energy transfer is completely characterized by the atomic energy-loss differential cross section $f(W, E) \in \mathbb{R}^+$, $W \in [0, E]$ and its moments

$$\sigma_E^{(n)} = \int_0^E W^n f(W, E) dW, \quad n \geq 0.$$

If there are N atoms per cm^3 , then $(N\sigma_E^{(0)})^{-1}$ is the mean free path length, $\sigma_E^{(1)}/\sigma_E^{(0)}$ the mean energy loss in a collision, and $\sigma_E^{(k)}/\sigma_E^{(0)}$, $k \geq 2$, the k -th moment of the energy loss in a collision. Under idealised assumptions that N is sufficiently large and that interactions occur independently, the energy loss per unit track length is well-approximated by $N\sigma_E^{(1)} + Z(N\sigma_E^{(2)})^{1/2}$, where $Z \sim \mathcal{N}(0, 1)$. Indeed, this is just a consequence of the central limit theorem. Thus, for the SDE we choose $\varsigma_1(x) = N\sigma_E^{(1)}$ and $\varsigma_2(x) = (N\sigma_E^{(2)})^{1/2}$. Explicit values of $N\sigma_E^{(1)}$ and $N\sigma_E^{(2)}$ are given by the well-established theory of the Bethe–Bloch formula which is discussed in detail in the following two sections.

4.1.1 The Bethe–Bloch formula for mean energy loss

The current state of the art model for mean energy loss from inelastic collisions is given by the Bethe–Bloch formula, along with its corrections. This quantum theory of stopping, originally due to Bethe, is based on the relativistic plane-wave Born approximation (Fano 1963). The Bethe–Bloch formula without corrections (Gottschalk 2018, Section 3.2 and Appendix D) per unit track length reads

$$\varsigma_1(x) = 0.3072 \frac{Z\rho}{A\beta^2} \left(\log \left(\frac{2m_e c^2 \beta^2}{I(1-\beta^2)} \right) - \beta^2 \right) \frac{\text{MeV}}{\text{cm}}, \quad (3)$$

with

$$\beta^2 = \frac{(2m_p c^2 + E)E}{(m_p c^2 + E)^2},$$

where ρ is the density of the medium in g/cm^3 , Z is the atomic number of the medium, A is the atomic mass of the medium, m_p is the mass of a proton, m_e is the mass of an electron, c is the speed of light, and I is the mean excitation energy of the medium. Importantly, this derivation assumes the idealised setting mentioned in the previous section. To account for this, several additional correction terms exist which result in a more accurate model. However, since the scope of this article is modeling the energy deposition of 100–150 MeV protons, we exclude correction terms due to them having little impact in this setting, as justified below.

There are four correction terms to the Bethe–Bloch formula, known as the shell, density, Lindhard–Sørensen, and the Barkas correction term, respectively. Their details can be found in equation Sections V–VII of Salvat (2022). All are known to be negligible in the proton energy range of clinical interest (Bischel & Hiraoka 1992, Mbagwu 2025, Salvat 2022, Salvat et al. 2022).

To extend (3) to materials consisting of more than one element we use the so-called Bragg-additivity rule. This assumes that the material can be treated as a uniform mix of each of its constituting elements, and that interactions are independent between elements. In this case, the Bethe–Bloch formula reads (Gottschalk 2018, Eq. (8))

$$\varsigma_1(x) = 0.3072 \sum_{i=1}^n \frac{Z_i \rho_i}{A_i \beta^2} \left(\log \left(\frac{2m_e c^2 \beta^2}{I(1 - \beta^2)} \right) - \beta^2 \right) \frac{\text{MeV}}{\text{cm}}, \quad (4)$$

where ρ_i , Z_i and A_i are the respective density, atomic number, and atomic mass of element i in the medium.

Lastly, we note that due to the idealised setting used to derive the Bethe–Bloch formula, equation (3) performs poorly when E is close to 0. Indeed, (3) tends to $-\infty$ as $E \rightarrow 0$. To account for this problem, for the results presented in Section 6, protons are absorbed upon reaching a kinetic energy of 0.05 MeV and their remaining energy is deposited at their current position. The choice of absorption energy threshold was determined by numerical evaluation of or implementation of (4) to ensure non-negative values, and is low enough that the remaining proton range is below 0.1 mm. Hence, the output of our simulations is unaffected for all practical purposes. An alternative approach using a logarithmic transform of the energy to guarantee non-negative energy for all track length has been considered in Chronholm & Pryer (2025).

4.1.2 Energy straggling

The original derivation of $N\sigma_E^{(2)}$ dates back to Bohr (Bohr 1987, Eq. (3.4.5)). However, this approach neglects the binding of atomic electrons and assumes interactions with non-relativistic free electrons at rest. A more accurate formula based on the relativistic plane-wave Born approximation (Salvat et al. 2022, Jackson 1975) reads

$$\varsigma_2(x)^2 = \frac{4\pi N_A Z \rho}{A} (\alpha \hbar c)^2 \left(\gamma^2 \left(1 - \frac{\beta^2}{2} \right) \right) \frac{\text{MeV}^2}{\text{cm}}, \quad (5)$$

where N_A is Avogadro’s constant, γ is the Lorentz factor, α is the fine structure constant, \hbar is the reduced Planck constant, and all other variables are as in Section 4.1.1. Identically to (3), due to the idealised setting assumed when deriving (5), an accurate formula for ς_2 requires additional correction terms. However, for the clinical energy range of protons with 0–150 MeV, the results of Salvat et al. (2022) show that they have negligible impact when the atomic number of the material is sufficiently small (less than 40), and between a 1–5% impact for larger atomic numbers. Furthermore, since the effect of energy straggling is small in itself, these errors will be of an order of magnitude smaller when compared to the total energy loss.

Identically to (4), we extend (5) to materials consisting of more than one element using the Bragg-additivity rule. This reads

$$\varsigma_2(x)^2 = \sum_{i=1}^n \frac{4\pi N_A Z_i \rho_i}{A_i} (\alpha \hbar c)^2 \left(\gamma^2 \left(1 - \frac{\beta^2}{2} \right) \right) \frac{\text{MeV}^2}{\text{cm}}.$$

4.2 Elastic scattering

We recall from Section 2.1 that elastic scattering is divided into Coulomb and nuclear scattering events, and the interference between them. At small angles, the effect of elastic scattering is dominated by Coulomb contribution (Trkov & Brown 2018, Section 6.2.7). We recall that the SDE (1) models small angle elastic scattering through a diffusion on the sphere with volatility m . Thus, we fit m using a physics-based Coulomb scattering model which is described in detail in Section 4.2.1. The SDE (1) models large angle elastic scattering as a point process with rate σ_e and jump density π_e . Since no satisfactory theory exists to describe the contributions from nuclear and nuclear-Coulomb elastic scattering, these parameters are fitted from the nuclear data libraries *ENDF/B-VIII.1* and *JEFF-4.0* which is described in detail in Section 4.2.2.

4.2.1 Molière’s theory for small-angle elastic scattering

The state of the art for modelling Coulomb scattering is given by the theory of Molière (Bethe 1953). The scattering density derived by Molière’s has a Gaussian mode, but tails which are much heavier than Gaussian (Gottschalk 2018). Thus, we model small-angle elastic Coulomb scattering by taking a Gaussian approximation to Molière’s distribution. Specifically, we use the Lynch–Dahl approximation to Molière multiple scattering (Lynch & Dahl 1991, Eq. (7)) which is given as follows. Consider a proton with configuration $x = (E, R, \Omega) \in \mathcal{C}$ traveling through a medium consisting of a single element. Transforming to spherical coordinates such that Ω maps to $(1, 0, 0)$, after a path length z cm, the azimuthal angle is uniform in $[0, 2\pi]$ and the polar angle is the absolute value of a Gaussian with mean 0 and standard deviation σ_E given by:

$$\begin{aligned} \chi_c^2 &= \frac{0.157Z(Z+1)z}{A\rho(pv)^2}, \\ \chi_\alpha^2 &= 2.007 \times 10^{-5} Z^{2/3} \frac{1 + 3.34(Z\alpha/v)^2}{(pc)^2}, \\ w &= \frac{\chi_c^2}{2\chi_\alpha^2(1-F)}, \\ \sigma_E &= \sqrt{\frac{\chi_c^2}{1+F^2} \left(\frac{1+w}{w} \log(1+w) - 1 \right)}, \end{aligned}$$

where p is the momentum in MeV/ c , v the particles velocity, and all other parameters are as in Section 4.1. Note that the corresponding formula of Lynch & Dahl (1991) is missing the square root on the final line. Here, $F \in (0, 1)$ is a truncation parameter describing the central fraction of the Coulomb scattering distribution taken into account. This is necessary because

the tails of the distribution are not integrable, and we take $F = 0.98$. This approximation is accurate, and advantageous because it does not use the radiation length of the medium, which is difficult to measure precisely.

For compounds, an effective χ_c^2 is obtained by adding up all single-atom contributions, while an effective χ_α^2 is obtained via

$$\log(\chi_\alpha^2) = \frac{\sum_i \frac{Z_i(Z_i+1)}{A_i} \log(\chi_{\alpha,i}^2)}{\sum_i \frac{Z_i(Z_i+1)}{A_i}}.$$

To convert these Gaussian updates into a rigorous mathematical object for use in the SDE, we use that for small path length step sizes z cm, the Lynch–Dahl approximation is well-approximated by the increment of a spherical Brownian motion of size z and volatility

$$m(x) = \frac{\sigma_E}{z^{1/2}}.$$

For our simulations in Section 6, we take $z = 0.05$ cm and use Algorithm 1 of Mijatović et al. (2020) to compute fast and exact realisations of spherical Brownian motion.

4.2.2 Large angle elastic scattering via experimental data

As shown in Gottschalk (2018), the Lynch–Dahl approximation accurately models the effects of Coulomb elastic scattering for scattering angles up to $\sim 2.5\sigma_E$. Beyond that, the light Gaussian tails fall too quickly to match the heavier tails of Molière’s distribution. Computing these heavier tails requires an expensive root finding step (Gottschalk 2018, Eq. (19)). Molière’s theory also gives no insight into the contributions from nuclear and nuclear-Coulomb effects. Thus, we turn instead to nuclear data libraries to model elastic scattering angles above $2.5\sigma_E$. Also, we note that although $2.5\sigma_E$ is energy-dependent, we fix $2.5\sigma_E = 0.04$ radians as a cut-off throughout our simulations in Section 6. This is done for the sake of computational efficiency, since a change in $2.5\sigma_E$ requires a re-evaluation of the nuclear data. Furthermore, for energies above 10 MeV, 0.04 radians is a good approximation of $2.5\sigma_E$ in water.

Consider a proton with configuration $x = (E, R, \Omega) \in \mathcal{C}$ travelling through a medium consisting of a single element. We primarily use the *ENDF/B-VIII.1* data library, and refer to *JEFF-4.0* for elements not included in *ENDF/B-VIII.1*. For all elements except hydrogen, the scattering cross sections are given by *LAW=5* and *LTP=12* (Trkov & Brown 2018, Section 6.2.7). This format expresses the scattering cross section as

$$\sigma_c^c(\mu, E) = \sigma_R^c(\mu, E) + \sigma_{NI}^c(E)P_{NI}(\mu, E) \text{ barns/sr}, \quad (6)$$

where μ is the cosine of the polar scattering angle, $\sigma_R^c(\mu, E)$ is the differential Coulomb scattering cross section in the *center-of-mass* frame (conversion to the *lab* frame is given in Appendix A.1) given by Rutherford’s formula with electronic screening ignored, which reads

$$\sigma_R^c(\mu, E) = \frac{\eta^2}{k^2(1-\mu)^2},$$

where

$$k = \frac{A}{1+A} \sqrt{\frac{2m_p E}{\hbar^2 c^2}} \times 10^{-26}, \quad \eta = Z \sqrt{\frac{\alpha^2 m_p}{2E}} \times 10^6,$$

with parameters as in Section 4.1, and σ_{NI}^c, P_{NI} given by experimental data to account for nuclear and nuclear-Coulomb effects. Transforming (6) to a scattering rate per cm of path length travelled gives

$$\sigma_e(E) = \frac{2N_A \pi \rho}{A} \int_{-1}^{\cos(2.5\sigma_E)} (\sigma_R^c(\mu, E) + \sigma_{NI}^c(E) P_{NI}(\mu, E)) d\mu \times 10^{-24}. \quad (7)$$

The integral of $\sigma_R^c(\mu, E)$ is calculated explicitly. The integral of $P_{NI}(\mu, E)$ is calculated numerically by first fitting a cubic B-spline for $P_{NI}(\mu, E)$, then integrating the resulting spline. The density of the scattering angle is given by

$$\pi_e(E; \mu) = \frac{(\sigma_R^c(\mu, E) + \sigma_{NI}^c(E) P_{NI}(\mu, E))}{\int_{-1}^{\cos(2.5\sigma_E)} (\sigma_R^c(\mu, E) + \sigma_{NI}^c(E) P_{NI}(\mu, E)) d\mu}, \quad \mu \in [-1, \cos(2.5\sigma_E)]. \quad (8)$$

To simulate a realisation from this density, it is sufficient to know its cdf which is given by

$$\Pi_e(E; \nu) = \frac{\int_{-1}^{\nu} (\sigma_R^c(\mu, E) + \sigma_{NI}^c(E) P_{NI}(\mu, E)) d\mu}{\int_{-1}^{\cos(2.5\sigma_E)} (\sigma_R^c(\mu, E) + \sigma_{NI}^c(E) P_{NI}(\mu, E)) d\mu}, \quad \nu \in [-1, \cos(2.5\sigma_E)], \quad (9)$$

where the numerator is computed identically to (7). For the simulations presented in Section 6, both (7) and (9) are computed for a discrete lattice of energy values and linear interpolation is used to extend to the full energy range. Once a scattering angle is simulated, it is converted into the *lab* frame using (15).

For hydrogen, the scattering cross sections are given by $LAW=5$ and $LTP=1$. This format expresses the scattering cross section as

$$\sigma_e^c(\mu, E) = \sigma_R^c(\mu, E) + \sigma_N^c(\mu, E) \text{ barns/sr}, \quad (10)$$

where since the incident and target particles are identical, Rutherford's formula with electronic screening ignored now reads

$$\sigma_R^c(\mu, E) = \frac{2\eta^2}{k^2 (1 - \mu^2)} \left[\frac{1 + \mu^2}{1 - \mu^2} - \frac{1}{2} \cos \left(\eta \ln \frac{1 + \mu}{1 - \mu} \right) \right],$$

furthermore

$$\sigma_N^c(\mu, E) = \sum_{l=0}^{NL} \frac{4l+1}{2} b_l(E) P_{2l}(\mu) - \frac{2\eta}{1 - \mu^2} \text{Re} \left\{ \sum_{l=0}^{NL} \left[\begin{array}{l} (1 + \mu) \exp \left(i\eta \ln \frac{1 - \mu}{2} \right) \\ + (-1)^l (1 - \mu) \exp \left(i\eta \ln \frac{1 + \mu}{2} \right) \end{array} \right] \frac{2l+1}{2} a_l(E) P_l(\mu) \right\}, \quad (11)$$

where P_l is the Legendre polynomial of degree l , $a_l(E)$ and $b_l(E)$ are respectively complex and real coefficients derived from experimental data, and the value of NL represents the

highest partial wave contributing to nuclear scattering which is equal to 7 for the hydrogen dataset provided by the *ENDF/B-VIII.1* library. As before, transforming (6) to a scattering rate per cm of path length travelled gives

$$\sigma_e(E) = \frac{2N_A\pi\rho}{A} \int_{-1+\delta}^{\cos(2.5\sigma_E)} (\sigma_R^c(\mu, E) + \sigma_N^c(\mu, E))d\mu \times 10^{-24}, \quad (12)$$

where $\delta > 0$ is a user-defined truncation parameter required since the tail of the Rutherford cross section for identical particles as $\mu \rightarrow -1$ is not integrable (for the simulations presented in Section 6 we take $\delta = 1 + \cos(\pi - 0.2)$). Similarly, accounting for δ in the lower limit, the associated density and cdf of the scattering angle are given by (8) and (9) respectively. The coefficients $a_l(E), b_l(E)$ are given for a set of lattice points which we extend using a cubic B-spline. Moreover, for given coefficients $a_l(E), b_l(E)$, the integrals in (9) can be computed explicitly as shown in Appendix A.1. Finally, for compound materials, we again assume Bragg-additivity meaning the point process σ_e, π_e can be decomposed as the sum of n independent point processes, where process i corresponds to the elastic scattering due to atoms of element i .

4.3 Inelastic proton-nucleus collision and scatter

As before, consider a proton with configuration $x = (E, R, \Omega) \in \mathcal{C}$ travelling through a medium consisting of a single element. We recall from (1) that inelastic proton-nucleus interactions occur in the SDE at an element-dependent rate σ_{ne} , and the outgoing energy and angle of the proton after such an interaction is given by the density π_{ne} . There exists no satisfactory theory to describe the effects of these interactions, so we use experimental data to model σ_{ne} and π_{ne} . As for large elastic scattering, we use the *ENDF/B-VIII.1* and *JEFF-4.0* nuclear data libraries. These libraries use the Kalbach-Mann systematics representation to model inelastic proton-nucleus interactions (Kalbach 1988) which is given as follows. The scattering rate per cm of path length travelled, $\sigma_{ne}(E)$, is given for a lattice of points in \mathcal{E} which we fit to a cubic B-spline to extend to \mathcal{E} . Furthermore, for a given lattice point $E_i \in \mathcal{E}$, the marginal distribution of the outgoing energy, which we denote $\pi_{ne}(E_i; du)$, along with a fitted parameter for the outgoing angle density, denoted $r(E_i, u) \in [0, 1]$, are given for a lattice of points in $\mathcal{E} \setminus (E_i, \infty]$ which we extend to $\mathcal{E} \setminus (E_i, \infty]$ and $[0, 1]$ respectively using cubic B-splines. Finally, the distribution of the cosine of the polar scattering angle in the *center-of-mass* frame (conversion to the *lab* frame is given in Appendix A.1) given incident energy E and outgoing energy u is given by

$$\pi_{ne}(\mu|E, u) = \frac{a(E, u)}{2 \sinh(a(E, u))} (\cosh(a(E, u)\mu) + r(E, u) \sinh(a(E, u)\mu)),$$

where $a(E, u)$ is a known constant given in Section 6.2.2 of Trkov & Brown (2018). The cdf of this density is invertible, thus the outgoing angle, μ , can be simulated using

$$\begin{aligned} \mu &= (C + (C^2 - r(E, \mu)^2 + 1)^{1/2}) / (r(E, \mu) + 1), \\ C &= 2 \sinh(a(E, \mu))U + r(E, \mu) \cosh(a(E, \mu)) - \sinh(a(E, \mu)), \end{aligned}$$

with $U \sim \text{Unif}[0, 1]$. The setting of compound materials is handled identically to large elastic scattering (Section 4.2.2).

5 Comparison methods

To verify the results from the proposed model, the Monte Carlo simulation toolkit Geant4 (version 11.3) (Agostinelli et al. 2003) was used as the benchmark. Geant4 was selected for its flexibility, including the ability to enable or disable specific physical processes and customise physics lists. For this study, we have used the prebuilt `QGSP_BIC_EMZ` physics list, as it provides accurate proton transport modelling via the Binary Cascade model and includes the `EMZ` option, which offers the most precise electromagnetic physics list in Geant4, optimised for low-energy proton transport.

5.1 Geometry configurations

Both simulations were configured with identical parameters and tested using cubic homogeneous and heterogeneous phantoms. For the homogeneous phantom, a monoenergetic proton beam (energy of 100 or 150 MeV, nozzle radius of 5 mm, energy spread σ_E of 0.1 keV and radial dispersion σ_r of 0.05 rad) was directed perpendicularly into water, with no air gap between the source and the phantom. For the heterogeneous phantom, a 100 MeV proton beam with the same beam settings was used to irradiate a cubic phantom with 2 cm of bone, followed by water. The chemical compositions and densities for all materials are the same for Geant4 and the SDE model. For all cases, 1×10^6 protons were fired per run, and dose was scored in both cases using a 3D grid of 1 mm^3 voxels across the irradiated volume, enabling pointwise comparison of the resulting dose distributions. The SDE model requires angular limits for backscatter and Rutherford events, which were both set at 0.04 rad. Since the SDE model employs a fixed step length, this was set to 0.5 mm for all simulations. For consistency, the maximum step length in Geant4 was constrained to the same value to ensure a fair comparison in terms of time performance.

5.2 Quantitative analysis

For quantitative assessment, we used integral dose-depth curves, central-axis depth-dose distributions, and lateral profiles. For a more rigorous evaluation, a full 3D gamma analysis (Low 2010) was performed. The analysis was implemented using the `pymedphys` Python package, which incorporates methods presented in Wendling et al. (2007). Gamma analysis is a standard method in radiotherapy for comparing dose distributions, as it accounts for both dose differences and spatial discrepancies in a single metric, making it particularly suitable for validating novel dose calculation models.

In this analysis, the dose distribution from the SDE model is treated as the evaluated distribution, while the Geant4 output serves as the reference. For a pair of evaluated and reference points ($\mathbf{r}_e, \mathbf{r}_r$), the generalised Euclidean distance Γ in a combined dose–distance space can be calculated using the dose difference (DD) and distance-to-agreement (DTA) criteria:

$$\Gamma(\mathbf{r}_e, \mathbf{r}_r) = \sqrt{\frac{\|\mathbf{r}_e - \mathbf{r}_r\|_2^2}{\text{DTA}^2} + \frac{|D_e(\mathbf{r}_e) - D_r(\mathbf{r}_r)|^2}{\text{DD}^2}}. \quad (13)$$

Here, $D_e(\mathbf{r}_e)$ and $D_r(\mathbf{r}_r)$ are the dose values at the evaluated and reference points, respectively, and $\|\mathbf{r}\|_2$ denotes the usual Euclidean 2-norm of the vector \mathbf{r} . The dose difference

(DD) and distance-to-agreement (DTA) criteria define the acceptable tolerances for dose and spatial deviation. The DD criterion can be normalised either globally (relative to the maximum dose) or locally (relative to the dose at each reference point). In this study, the local normalisation method was used. A dose threshold of 1% of the maximum dose was applied to exclude low-dose noise, and the gamma analysis was performed with criteria of $DD = 1\%$ and $DTA = 2$ mm.

The gamma index γ for a given reference point \mathbf{r}_r is determined by searching over all evaluated points \mathbf{r}_e within a radius equal to the DTA. To reduce the influence of the discrete voxel grid, the gamma analysis algorithm in `pymedphys` employs on-the-fly linear interpolation between voxels, allowing γ to be evaluated at sub-voxel positions. This process is controlled by the interpolation fraction, which specifies the interpolation step size as a fraction of the DTA criterion. In this study, the interpolation fraction was set to 10, corresponding to a step size of 0.2 mm. This interpolation does not alter the underlying dose distributions, but enables a more accurate determination of the gamma index, which satisfies:

$$\gamma(\mathbf{r}_r) = \min_{\mathbf{r}_e: \|\mathbf{r}_e - \mathbf{r}_r\|_2 \leq DTA} \{\Gamma(\mathbf{r}_e, \mathbf{r}_r)\}. \quad (14)$$

A point is considered to pass if $\gamma(\mathbf{r}_r) < 1$ and fail otherwise. The overall agreement is expressed as the percentage of reference points that satisfy the gamma criterion. Pass rates are strongly influenced by the chosen DD/DTA criteria and the normalisation method. As a benchmark, universal tolerance limits recommended in Miften et al. (2018) specify a pass rate of $\geq 95\%$ using 3%/2 mm criteria with a 10% dose threshold under global normalisation.

6 Results and discussion

6.1 Proton transport in homogeneous medium

This first test involves the irradiation of a cubic water phantom with a size of $20 \times 20 \times 20$ cm³, subdivided into 1 mm³ cubic voxels in both the SDE and Geant4 models. From the 3D dose arrays, a central-axis 2D slice was extracted to visualise the overall dose distributions, which are shown in Figure 3 using a 100 MeV beam. The dose maps, plotted on a logarithmic scale, illustrate the strong agreement between the SDE and Geant4, including in low-dose regions where the SDE accurately captures lateral spread. The main differences are observed in the lowest dose values, corresponding to non-local dose deposits present only in the Geant4 maps. These arise from secondary particles, such as gammas and neutrons, which travel away from the primary beam and interact with atoms at distant locations, producing small, remote dose contributions that the current SDE model does not simulate.

Based on these findings, a more detailed comparative analysis was performed, including results from a 150 MeV proton beam to assess the SDE output at higher proton energies. The depth-dose curves shown in Figure 4a were obtained by integrating the 3D dose distribution over the cross sectional area to obtain a 1D Bragg peak. Deviations between the integrated depth-dose curves are below 3% for a 100 MeV beam and below 6.5% for a 150 MeV when evaluated pointwise before the Bragg peak. Beyond the peak, two factors lead to systematic differences between the models. First, the SDE model applies an energy threshold below

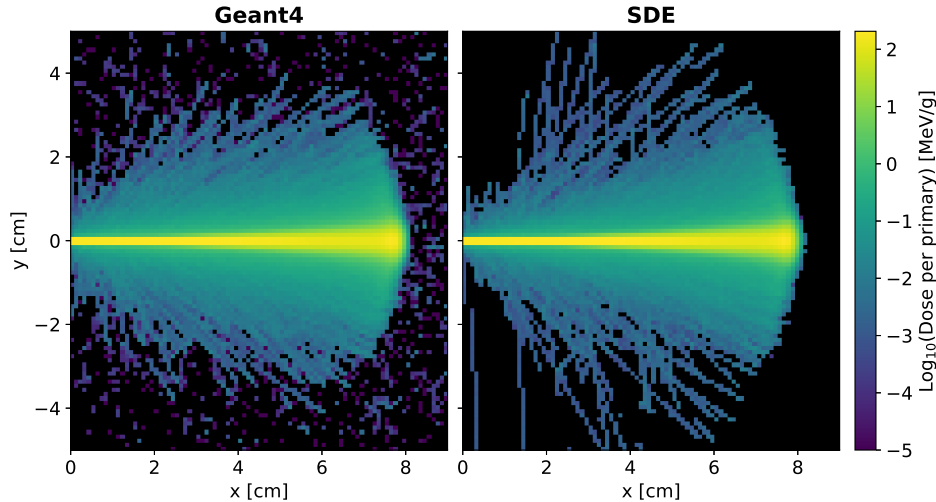


Figure 3: 2D central-axis dose distribution comparison using a monoenergetic 100 MeV proton beam in a homogeneous water phantom.

which proton transport is terminated, which causes the dose to fall off slightly faster than in Geant4. Second, because the SDE does not model dose contributions from secondary particles such as neutrons and gammas, it does not reproduce the remanent dose at remote locations predicted by Geant4. Together, these effects result in a steeper fall-off and zero dose deposition at greater depths in the SDE results. Nevertheless, the proton range is accurately reproduced, with R90 agreeing within less than 0.1 mm for 100 MeV and within 0.4 mm for 150 MeV. This evidences the accuracy in the electromagnetic processes modelled in our approach. Moreover, the percentage differences in the integrated depth-dose curves are highest at mid-depths and decrease towards the Bragg peak. This behaviour indicates that the SDE model achieves its best agreement with Geant4 in the high-dose region near the Bragg peak, where dose accuracy is most critical.

For a more detailed comparison of the core beam behaviour, differential depth-dose curves were obtained from the central voxels of the 3D dose arrays and are shown in Figure 4b. These curves are highly sensitive to local variations in scattering, energy loss and voxel sampling, which results in a higher overall percentage difference compared to integrated depth-dose curves, while remaining within 10% for 100 MeV and 20% for 150 MeV. Moreover, these curves are sensitive to the angular limits set in the SDE model for Rutherford and backscatter events. The agreement is highest at shallow depths, after which it starts decreasing. Overall, the trends suggests that the SDE model reproduces the core beam behaviour reliably, while minor discrepancies at depth are expected due to the differences in scattering modelling.

To further evaluate the beam’s lateral spread and its consistency with depth, Figures 5a and 5b show the lateral profiles at different depths for 100 and 150 MeV, respectively. The SDE model consistently reproduces the overall Gaussian beam shape, showing similar widths to Geant4 across all depths. This indicates that multiple scattering is modelled with high accuracy. Small, systematic overestimation of the absolute dose is confirmed in all profiles, as can be expected because Geant4 models many energy-dissipating processes neglected by the SDE, most notably a larger range of secondary particles. Despite this, the

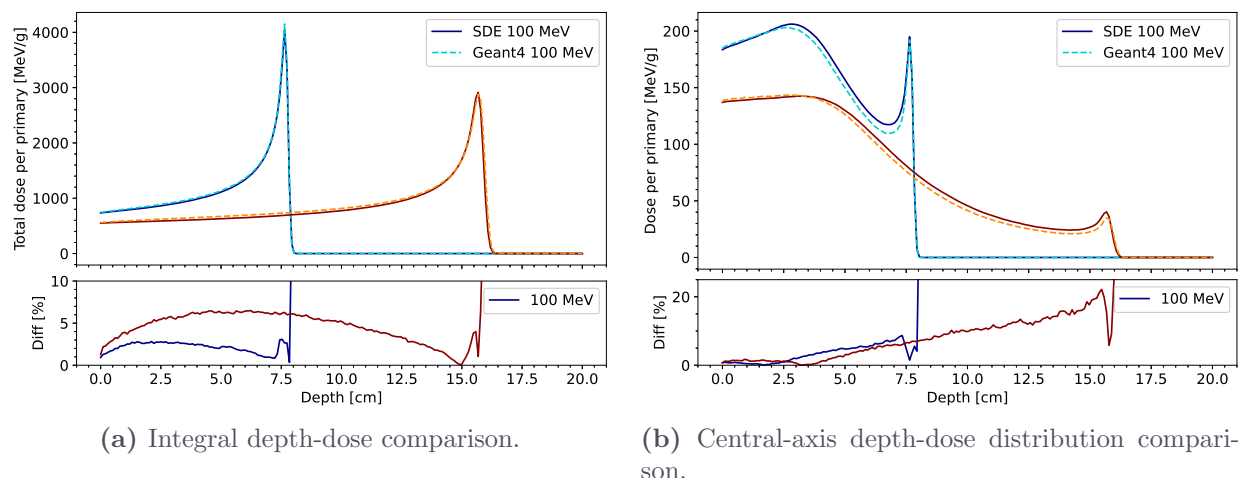


Figure 4: 1D comparison between SDE and Geant4 for two monoenergetic proton beams (100 and 150 MeV) in a homogeneous water phantom, including pointwise calculations for percentage dose differences in the lower subplots.

close match in profile widths demonstrates that the spatial dispersion of the beam is well captured, confirming the accuracy of the model in describing lateral transport.

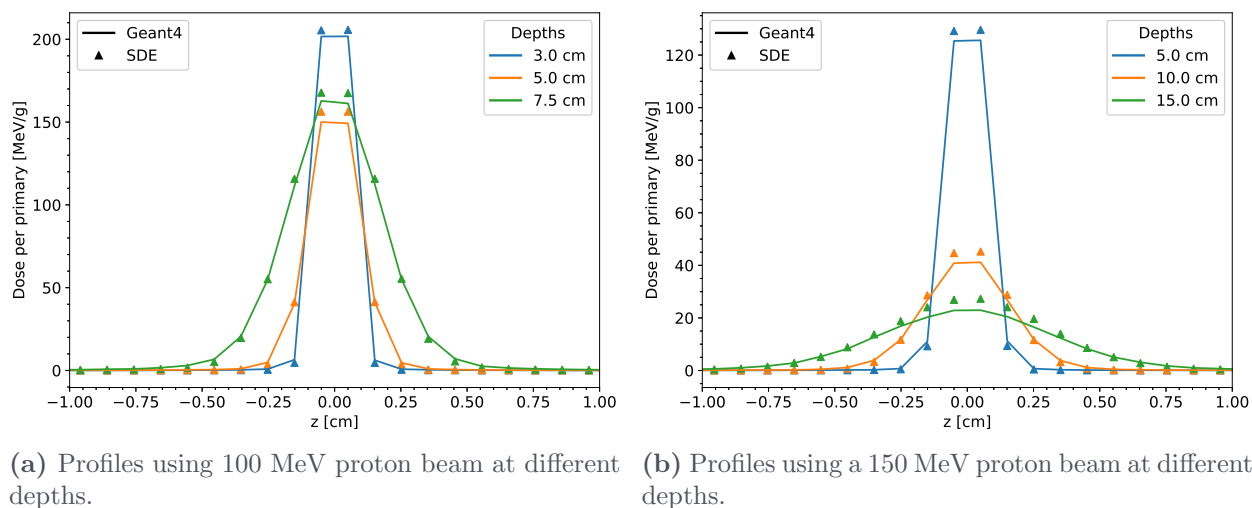
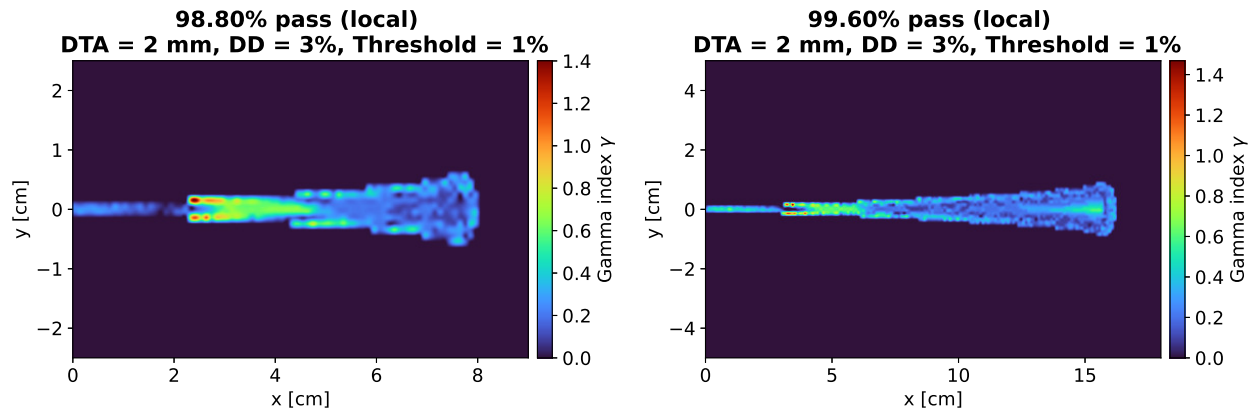


Figure 5: Lateral profile comparison between SDE (marker points) and Geant4 (solid lines) for two proton energies in a homogeneous water phantom.

To illustrate the potential of our model for clinical purposes, gamma analysis was performed in 3D for thorough comparison for the two proton energies under study. Figure 6 shows central-axis slices from the resulting 3D gamma index matrices for each proton energy under study, illustrating that the gamma indices remain well below unity throughout the high-dose region, confirming strong spatial and dosimetric agreement between the SDE model and Geant4. The largest discrepancies are confined to low-dose regions near the beam periphery, where secondary-particle effects, absent in the SDE model, contribute in Geant4. In addition, Table 1 presents the gamma pass rates for several commonly used criteria. Pass

rates exceed 98% for all evaluated criteria, reaching 100% under the conventional 3%/2 mm condition for a 10% dose threshold. These results demonstrate that the SDE model achieves clinically acceptable agreement with Geant4.



(a) Gamma distribution using 100 MeV proton beam. (b) Gamma distribution using 150 MeV proton beam.

Figure 6: Central-axis gamma index matrices for two proton beam energies in homogeneous water phantom.

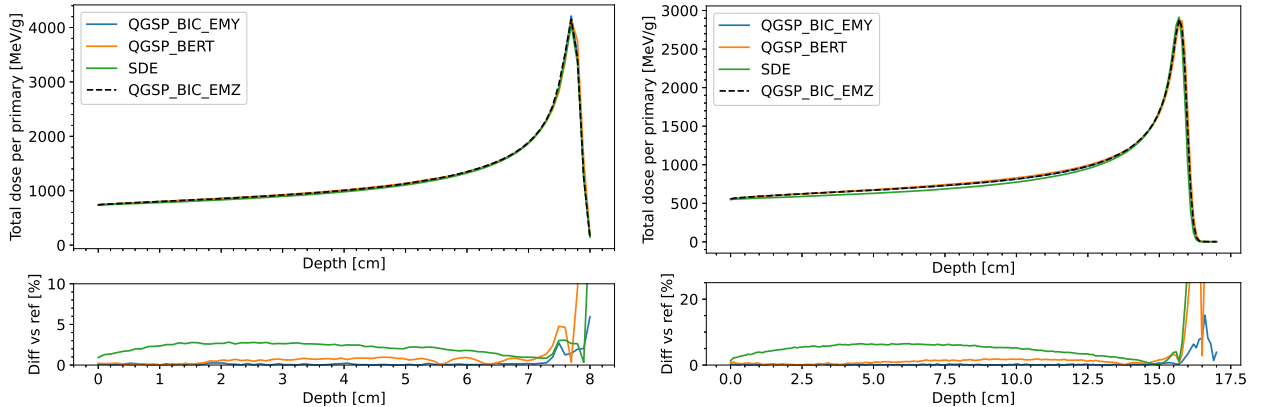
Energy (MeV)	DD (%)	DTA (mm)	Threshold (%)	Norm. Method	Pass rate (%)
100	3	2	10	global	100
	3	2	10	local	100
	3	2	1	local	98.80
	2	1	1	local	98.17
150	3	2	10	global	100
	3	2	10	local	100
	3	2	1	local	99.60
	2	1	1	local	99.26

Table 1: Gamma analysis pass rates in homogeneous water phantom using two monoenergetic proton energies.

6.2 Comparison against different Geant4 physics lists

To contextualise the observed differences between the SDE model and Geant4, Figure 7 compares integral depth-dose curves obtained with different Geant4 physics lists that are commonly used for proton therapy calculations (QGSP_BIC_EMZ, QGSP_BIC_EMY and QGSP_BERT). Comparisons are shown for 100 MeV (Fig. 7a) and 150 MeV (Fig. 7b) proton beams, with the percentage differences calculated with respect to the reference physics list, QGSP_BIC_EMZ. The SDE curve is also included for reference, illustrating that the deviation between the SDE

model and the reference Geant4 configuration lies within the typical range of variability observed among Geant4 physics lists. Notably, while the SDE model exhibits the largest discrepancies in the low-dose tail of the Bragg curve, agreement in the high-dose region near the peak remains within the inter-list variations of Geant4. These results reinforce the physical consistency of the SDE model, while future efforts will focus on reducing these discrepancies through the implementation of secondary particle modelling.



(a) Depth-dose curves using a monoenergetic 100 MeV beam.

(b) Depth-dose curves using a monoenergetic 150 MeV beam.

Figure 7: Integral depth-dose comparison between different Geant4 physical models and the SDE model. The reference physics list (QGSP_BIC_EMZ) is shown in dotted lines.

6.3 Proton transport in heterogeneous medium

To assess the capability of the proposed model to handle material heterogeneities and associated range shifts, a second test was conducted using a cubic phantom containing a 2-cm-thick bone insert positioned at the beam entrance. All other parameters were kept identical to those of the homogeneous water case described in the previous section. Figure 8 presents the 1D comparisons for 100 and 150 MeV monoenergetic proton beams. The integrated depth-dose curves show excellent agreement between the two models, with calculated range differences below 0.1 mm for 100 MeV and 0.4 mm for 150 MeV. Along the central axis, the dose deviations within the bone region remain below 5%. Interestingly, this region exhibits a slight underestimation by the SDE model, in contrast to the homogeneous case, where an overall dose overestimation was observed. As illustrated by the lateral profiles in Figure 9, this underestimation is confined to the bone region of the phantom. Beyond the bone interface, where the medium returns to water, both models regain strong agreement at mid-depths, while the SDE again shows an overestimation near the Bragg peak.

To further quantify agreement, a gamma analysis was performed for both beam energies in the heterogeneous configuration, as shown in Figure 10 and summarised in Table 2. For clinically relevant criteria (3%/2 mm, 10% dose threshold), pass rates exceeded 99%, indicating strong consistency between SDE and Geant4 dose distributions. Even when applying more strict criteria (2%/1 mm, 10% dose threshold), the pass rates remained above 97%. Spatially, the bone region shows gamma indices close to but below 1 for the 3%/2

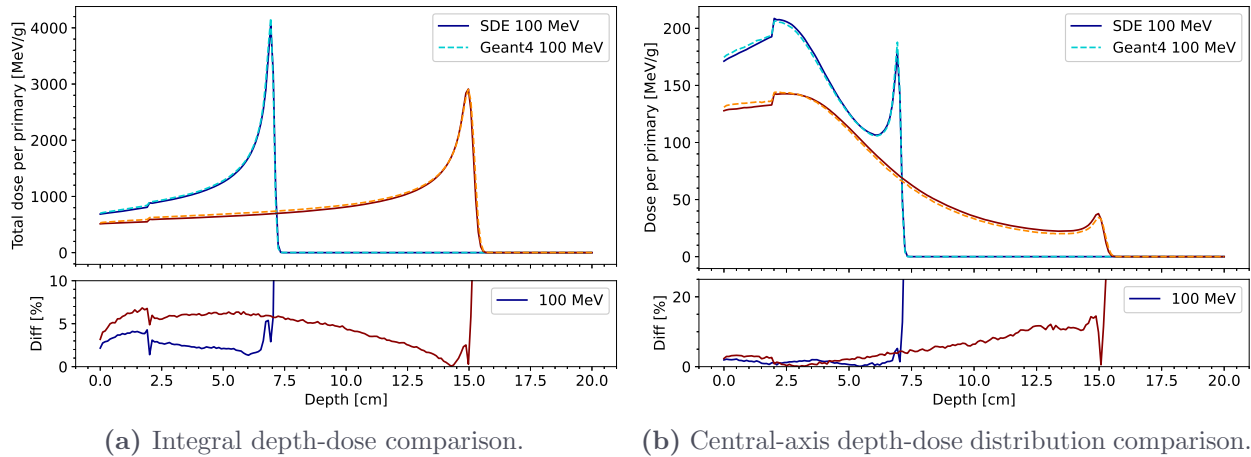


Figure 8: 1D comparison between SDE and Geant4 for two monoenergetic proton beams (100 and 150 MeV) in a heterogeneous phantom with a 2-cm bone layer. Lower subplots show pointwise percentage dose differences.

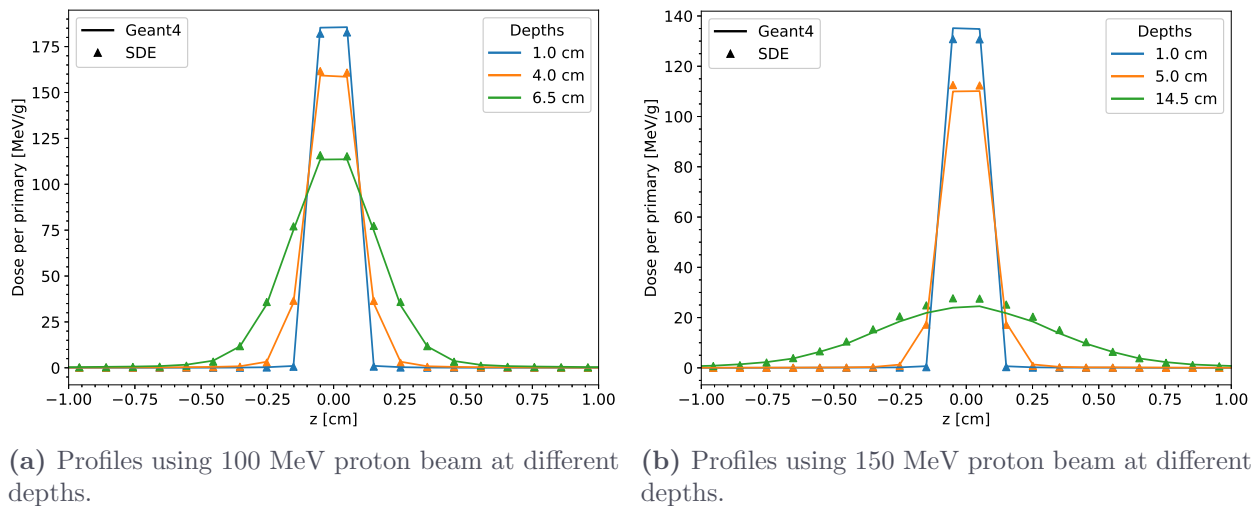
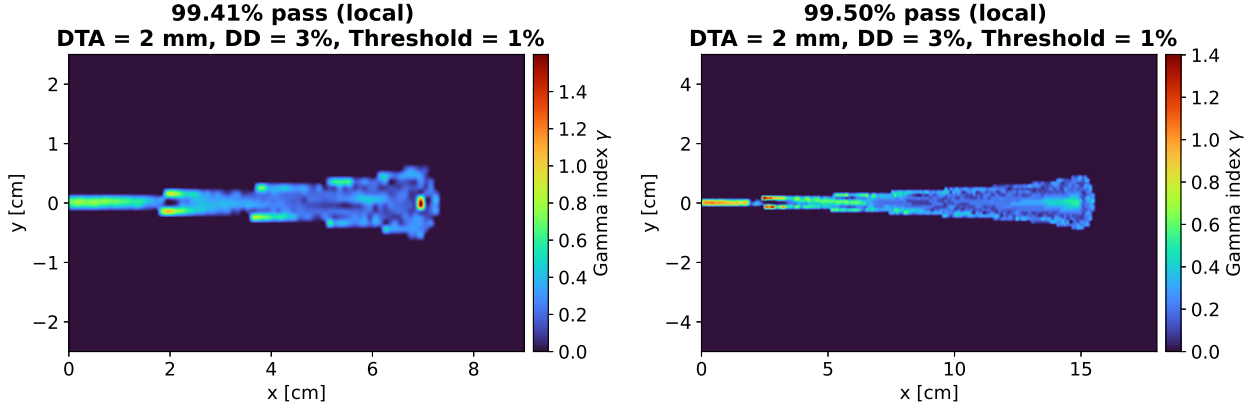


Figure 9: Lateral profile comparison between SDE (marker points) and Geant4 (solid lines) for two proton energies in a heterogeneous phantom. The profile at 1 cm corresponds to the bone region.

mm criterion, indicating that the agreement between the SDE and Geant4 remains within acceptable limits even in high-density regions. However, for more stringent criteria, some voxels in the bone region begin to fail, suggesting that further refinement may be needed to improve accuracy in high-density media.

6.4 Dose distribution in low density materials

The SDE underestimates the radial spread of dose in low-density media, such as air, due to the fact that it does not track ionisation electrons. Instead, the energy which would give rise to these electrons is deposited locally at the position of the primary proton. Ionisation electrons can travel a long distance when the density of the medium is low, resulting in a



(a) Gamma distribution using 100 MeV proton beam. (b) Gamma distribution using 150 MeV proton beam.

Figure 10: Central-axis gamma index matrices for 100 MeV and 150 MeV pristine proton beams in heterogeneous phantom.

Energy (MeV)	DD (%)	DTA (mm)	Threshold (%)	Norm. Method	Pass rate (%)
100	3	2	10	global	99.53
	3	2	10	local	99.53
	3	2	1	local	99.41
	2	1	1	local	97.52
150	3	2	10	global	99.62
	3	2	10	local	99.38
	3	2	1	local	99.50
	2	1	1	local	98.86

Table 2: Gamma analysis pass rates in heterogeneous phantom using two monoenergetic proton energies.

discrepancy in the radial spread of dose between the SDE output and a Geant4 benchmark.

We illustrate this effect by considering the same bone-water phantom as in Section 6.3 with a 5 cm air gap between the nozzle and the bone layer. Integral depth-dose curves (Figure 11a) show good overall agreement between the SDE and Geant4, although slight discrepancies are observed at shallow depths, with differences approaching 20%. Central-axis depth-dose curves (Figure 11b) indicate that dose differences exceed 20% within the air region. We confirmed this by changing the electron production cut in Geant4 from the default value of 1 mm to a very large value (100 cm), the effect of which is for Geant4 to neglect these electrons and instead deposit their dose locally at the position of their creation. This removed the discrepancy, producing results similar to the SDE output.

Despite this discrepancy, the proton range agreement between the SDE and Geant4 remains within 0.2 mm, and lateral spread maintains good agreement in the denser materials, as seen in Figure 12a, which demonstrates no change in bone or water regions. However, at the air depth (2.5 cm), the lateral profile shows overestimation at the beam centre, consistent

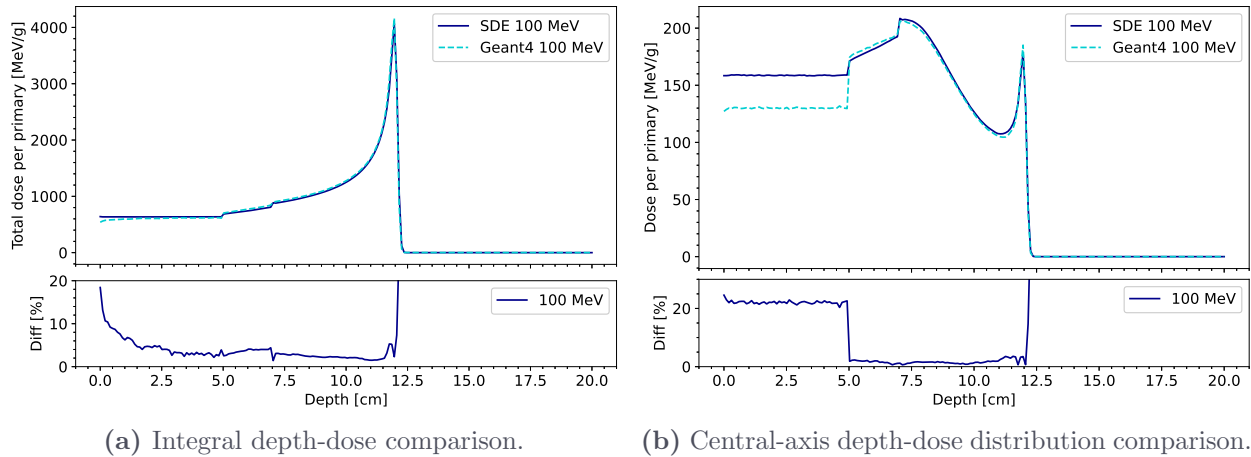


Figure 11: 1D comparison between SDE and Geant4 for a 100 MeV beam in a heterogeneous phantom with a 2-cm bone layer and an additional 5 cm air gap at the beam entrance. Lower subplots show pointwise percentage dose differences.

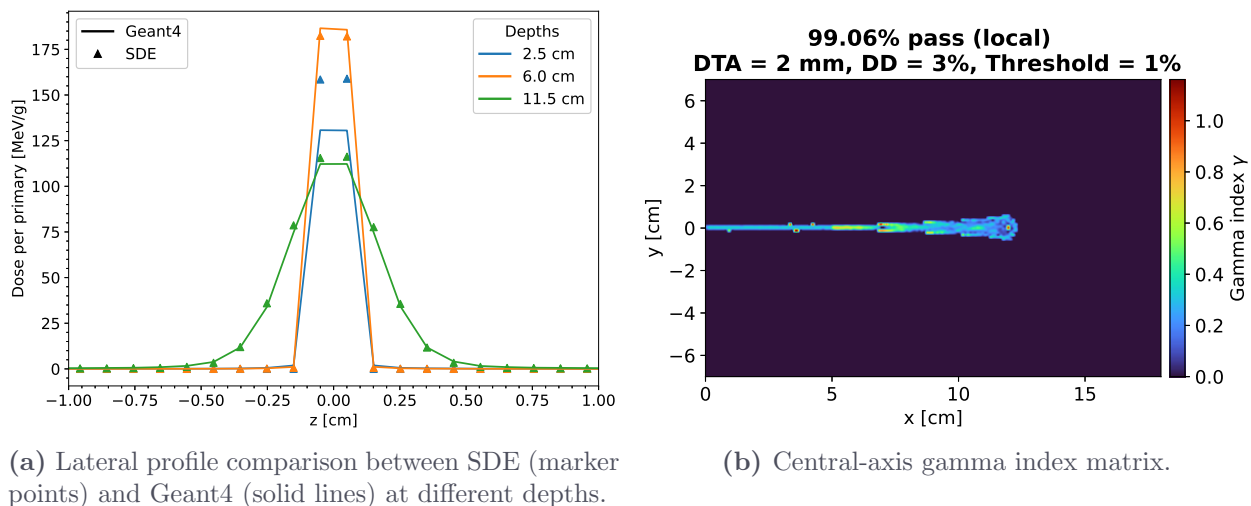


Figure 12: Further comparisons performed for a 100 MeV beam in a heterogeneous phantom, adding a 5 cm air gap before the phantom. The profiles at 2.5, 6.0 and 11.5 cm correspond to air, bone and water regions.

with the observed dose difference. Furthermore, 3D gamma analysis retains pass rates above 99% under strict criteria (3%/2 mm, 1% dose threshold), and the air region does not fail the gamma test, as seen in Figure 12b. Gamma analysis passes even in air because the region in which the SDE overestimates dose is very highly localised to the central voxel of the beam. Hence, a strict 2 mm comparison radius suffices to smooth out its effect.

These findings indicate that the SDE model underestimates dose in low-density materials, but clinical impact is limited since treatment-relevant doses are delivered to tissue rather than air gaps. For organs with significant air volumes, such as lungs, the resulting discrepancy could be relevant. Future work could address this by incorporating a mathematical description of electron diffusion in low-Z materials, rather than tracking individual electrons

as in Geant4.

6.5 Simulation time comparison

All simulations were executed on a single core of a MacBook Pro equipped with an Apple M2 Max chip, using 1×10^6 primary protons. The SDE model required 57.6 s to simulate 100 MeV protons a homogeneous water phantom and 60.5 s in a heterogeneous phantom, compared to 252.8 s and 247.2 s with Geant4 (QGSP_BIC_EMZ), representing a $4.1 \times$ and $4.4 \times$ speed improvement, respectively. At higher energies, these gains were more pronounced: the SDE model took 102.2 and 103.8 s for homogeneous and heterogeneous phantoms at 150 MeV, while Geant4 required 571.0 and 511.6 s with Geant4, corresponding to a 4.9 - $5.6 \times$ increase in computational efficiency. These factors do not vary significantly when using alternative Geant4 physics lists such as QGSP_BERT or QGSP_BIC_EMY, indicating that the observed speed advantage of the SDE model is largely independent of the specific physics configuration employed. Importantly, the SDE framework can be readily adapted for parallel execution across multiple cores, a strategy commonly used to accelerate Monte Carlo simulations, suggesting even greater performance potential without fundamental code modifications.

7 Conclusions

This study presents the first comprehensive validation of the SDE model for proton dose calculation, benchmarked against Geant4 in both homogeneous and heterogeneous phantoms. The model reproduces depth-dose curves, lateral spread, and 3D gamma indices with deviations that are comparable to those observed among various Geant4 physics lists. Additionally, the SDE model demonstrates a considerable computational speed advantage, which becomes more pronounced at higher proton energies. The implementation is readily parallelisable, which will allow for further speed increase. Future work will focus on simplified modelling of secondary particle contributions and optimisation of the source code for clinical use. Overall, these findings identify the SDE approach as a promising, fast and accurate alternative to conventional Monte Carlo simulations in proton therapy.

A Appendix

A.1 Angle conversion between reference frames

During the collision of a two-body system between a proton of mass m_1 and a target nucleus of mass m_2 , the angular distribution of the outgoing proton is obtained from nuclear data, which is often reported in the center of mass (CM) reference frame. Hence, it is necessary to perform a transformation of the angles to the lab (L) frame for use in the present model. Let v_{1L} and v_{1C} be the initial proton velocities in the lab and CM frames respectively, and v'_{1L} and v'_{1C} the final velocities in the respective frames. In general, the expression for the angle θ_L in the lab frame in terms of the angle θ_{CM} in the center of mass frame, bearing in mind relativistic effects, is given by

$$\tan \theta_L = \frac{\sin \theta_{CM}}{\gamma_u \left(\cos \theta_{CM} + \frac{u}{v'_{1C}} \right)}, \quad (15)$$

where u is the velocity of the center of mass of the two-body system and $\gamma_u = 1/\sqrt{1-u^2}$. If the kinetic energy K of the proton is known, then its total energy E_{1L} and momentum p_{1L} can be calculated using

$$\begin{aligned} E_{1L} &= K + m_1, \\ p_{1L} &= \sqrt{E_{1L}^2 - m_1^2}. \end{aligned}$$

In addition, u is also defined from these quantities, as it is not dependent on the nature of the collision:

$$u = \frac{p_{tot}}{E_{tot}} = \frac{p_{1L}}{E_{1L} + m_2}.$$

Given that we need an expression for the final proton velocity in the CM frame, we use the Lorentz velocity transformation

$$v'_{1C} = \frac{v'_{1L} - u}{1 - uv'_{1L}} = \frac{p'_{1L} - uE'_{1L}}{E'_{1L} - up'_{1L}}.$$

For the elastic case, the proton velocity remains the same before and after the collision in the CM frame, thus, we may use $p'_{1L} = p_{1L}$ and $E'_{1L} = E_{1L}$ with the definitions given earlier. For the inelastic case, there will be an associated proton energy loss E^* , meaning that

$$\begin{aligned} E'_{1L} &= E_{1L} - E^*, \\ p'_{1L} &= \sqrt{E'_{1L}^2 - m_1^2}. \end{aligned}$$

The outgoing proton energy can also be obtained from the nuclear database in the CM frame (referred to as E'_{1C}). To transform the energy back to the lab frame, the inverse Lorentz transformation can be used:

$$E'_{1L} = \gamma_u \left(E'_{1C} + u \cos(\theta_{CM}) \sqrt{(E'_{1C})^2 - m_1^2} \right). \quad (16)$$

A.2 Integration of (9) for Hydrogen elastic scattering

Firstly, to integrate $\sigma_R^c(\mu, E)$ we use that the anti-derivative of $\sigma_R^c(\mu, E)$, denoted $\sigma_R^{c,(1)}(\mu, E)$, is given by

$$\sigma_R^{c,(1)}(\mu, E) = \frac{2\eta^2\mu}{k^2(1-\mu^2)} - \frac{\eta}{2k^2} \sin \left(2\eta \ln \frac{1+\mu}{1-\mu} \right).$$

Next we move onto integrating $\sigma_N^c(\mu, E)$. The first term of (11) is the sum of polynomial functions whose integral is clear. For the second term, first note that by repeated integration by parts, for any $n+1$ -fold integrable function f ,

$$\int_0^\nu f(\mu)\mu^n d\mu = (-1)^{n+1}n!f^{(n+1)}(0) + \sum_{i=0}^n \frac{(-1)^i f^{(i+1)}(\nu)\nu^{n-i}n!}{(n-i)!},$$

where $f^{(i)}$ is the i th anti-derivative of f . This and the fact that σ_N^c is even in μ implies the integral of the second term can be written in terms of the antiderivatives of

$$f_{\pm}^{\cos}(\mu) = \frac{1}{1 \pm \mu} \cos \left(\eta \ln \frac{1 \pm \mu}{2} + C \right),$$

where the constant C is precisely the polar angle of the coefficient $a_l(E)$. More generally, let

$$f_{\pm}(\mu) = \frac{c_1}{1 \pm \mu} \cos \left(\eta \ln \frac{1 \pm \mu}{2} + C \right) + \frac{c_2}{1 \pm \mu} \sin \left(\eta \ln \frac{1 \pm \mu}{2} + C \right).$$

Using a $u = \ln((1 \pm \mu)/2)$ substitution along with integration by parts we obtain the recursive formula

$$\begin{aligned} f_{\pm}^{(n)}(\mu) &= (1 \pm \mu)^{n-1} \left(c_{\pm,n}^{\cos} \cos \left(\eta \ln \frac{1 \pm \mu}{2} + C \right) + c_{\pm,n}^{\sin} \sin \left(\eta \ln \frac{1 \pm \mu}{2} + C \right) \right), \\ c_{\pm,n+1}^{\cos} &= \frac{\pm(n c_{\pm,n}^{\cos} - \eta c_{\pm,n}^{\sin})}{(n^2 + \eta^2)}, \quad c_{\pm,n+1}^{\sin} = \frac{\pm(\eta c_{\pm,n}^{\cos} + n c_{\pm,n}^{\sin})}{(n^2 + \eta^2)}, \\ c_{\pm,0}^{\cos} &= c_1, \quad c_{\pm,0}^{\sin} = c_2. \end{aligned}$$

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Data sharing is not applicable to this article as no new data were generated or analysed.

Supplementary material

All of the results presented in this work can be replicated using the code available at <https://github.com/JereKoskela/proton-beam-sde>, which contains the SDE model source, the Geant4 models and Python scripts to generate the figures.

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