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A breakdown of the pseudo-deterministic transport variance reduction method : formalization and usage considerations

Valentin Champciaux[a], Juan-Carlos Garcia-Hernandez[a,*], Mathieu Agelou[a]

[a] *Université Paris-Saclay, CEA, List, F-91120, Palaiseau, France*

Abstract

The pseudo-deterministic (or simply deterministic) transport method is used in Monte Carlo particle transport problems to increase the sampling of a region in space that particles have a low probability of reaching. Although it has been used by many authors over the years, mainly due to its implementation in the code MCNP which itself has been extensively validated, to our knowledge, a proof of the unbiasedness of the method has never been published.

This article thus provides a comprehensive mathematical description of the pseudo-deterministic transport method, built from simple transformations of a given random variable representing an arbitrary physical quantity of interest. Some considerations are made for the handling of potential secondary particles created during the interaction process, and of specific estimators such as pulse height or energy spectrum.

This description should allow for a better understanding of the technique, including its possible uses and limitations, and can be used as a reference by both simulation code users and developpers looking to implement pseudo-deterministic transport in their code.

Keywords: monte carlo, particle transport, simulation, pseudo-deterministic transport, variance reduction, DXTRAN

*Corresponding author

Email addresses: valentin.champciaux@cea.fr (Valentin Champciaux), juan-carlos.garcia-hernandez@cea.fr (Juan-Carlos Garcia-Hernandez), mathieu.agelou@cea.fr (Mathieu Agelou)

1. Introduction

The pseudo-deterministic transport method is meant to improve the sampling of a region in space that particles have a low probability of reaching, and therefore improve the efficiency of estimations made in this area. It is used whenever a scattering interaction occurs, at which point a new particle, called "deterministic", is created. Its direction is sampled towards a user-defined sphere, arbitrarily placed in space, and the distance travelled before the next interaction is sampled such that it is large enough to reach the sphere. This makes it possible to bring a particle to the area of interest for every scattering event occuring during the simulation. Estimations are supposed to remain unbiased by :

- Appropriately weighting the deterministic particle, depending on the probability of being scattered towards the sphere and then reaching it.
- Killing the original particle if it enters the sphere during the step following the scattering event (which means giving zero weight to any subsequent contribution to an estimator).

The most detailed description of this method can be found in the MCNP code documentation [1], due to the implementation in MCNP of a version of the pseudo-deterministic transport called DXTRAN. This description, although useful for MCNP users, could be considered incomplete : while it gives the general recipe for applying the technique to particle transport, such as the deterministic particle weight or the conditions that lead to killing the original particle, it doesn't provide a complete and formal mathematical description of the method, including a proof of its unbiasedness regarding the various estimations that can be made while using this technique. No mention is made, either, of the secondary particles potentially created by the interaction, and thus questions can arise : assuming this technique is applied to the Compton scattering of a photon and creates a new deterministic photon, what of the recoil electron ? Is it necessary to create a second one, and if so what would be its energy, direction and weight ?

The MCNP documentation is generally used as a basis for other descriptions of the method found in the litterature, and, to our knowledge, no formal description and proof of its unbiasdness has been published yet. This, however, could be necessary for implementing the method in any Monte Carlo simulation code used to solve problems that would require a better sampling

of a remote or shielded area, such as the calculation of the out-of-field dose in radiotherapy. This article thus aims to provide a proper mathematical description of the pseudo-deterministic transport method, by building the technique from simple mathemathical transformations of the random variable used in an arbitrary estimation of a physical quantity.

2. Sampling of a scattering event

Let us consider a very general case of a particle transport Monte Carlo model, in which the random variable Y represents any physical quantity of interest. From that model we can draw samples y_i of Y, which is equivalent to simulating particle tracks and scoring the adequate quantities. This allows an estimation of some of the properties of Y by using the appropriate estimator, such as using the mean deposited energy over N particle tracks to estimate its expected value. Note that even though we refer to this process as "sampling" the random variable, it could instead be called "generating a value according to its probability density function", while keeping the word "sampling" for directly drawing samples from a known probability density function. Both will be called "sampling" in this paper, but it must be kept in mind that this sampling will generally be done indirectly as the probability density function of the variable is usually unknown.

Transporting a particle, or drawing a sample of Y, is done by sampling a series of interactions between which the particle travels in straight lines called steps. Both the outcome of interactions and the travelled distance during a step are random and can be represented by random variables which probability density functions are determined by physical laws and considered to be known at least approximately in a simulation code.

In the context of particle transport, the variable Y can be expressed as a function of every physical event or random process taking place during the particle track, expressed as variables X_0 to X_n, such that :

$$Y = h(X_0, X_1, \ldots, X_{n-1}, X_n) \tag{1}$$

Assuming a scattering event takes place during the particle track between the two random processes X_k and X_l, then we can write

$$Y = h(X_0, \ldots, X_k, \overrightarrow{\Omega}, X, X_l \ldots, X_n) \tag{2}$$

where $\overrightarrow{\Omega}$ is the random variable associated to the scattering direction and X is the distance travelled before the next interaction. The variables X_0 to

X_k will be referred to as $\overrightarrow{X_0}$ and the variables X_l to X_n as $\overrightarrow{X_n}$, such that we have

$$Y = h(\overrightarrow{X_0}, \overrightarrow{\Omega}, X, \overrightarrow{X_n}) \tag{3}$$

The function h depends on how quantities of interest are scored during the particle transport. In the case of the energy deposited by a source particle in some volume, a sample of Y is the sum of all instances of energy deposit in said volume during the particle track. In this case, Y can be written as the sum of quantities scored before and after any scattering event, such that

$$Y = g_0(\overrightarrow{X_0}) + g(\overrightarrow{\Omega}, X, \overrightarrow{X_n}) = Y_0 + Y_n \tag{4}$$

The value of Y_0 is known from scoring quantities before the scattering event, while Y_n is computed by scoring values during and after the interaction. Note that even though Y_n only depends on $\overrightarrow{\Omega}$, X and $\overrightarrow{X_n}$, in practice, its sampling still requires the sampling of $\overrightarrow{X_0}$, as the probability density functions of random events are only known conditionally to the outcome of the previous event. In other words, to score the required quantitites after the scattering event, the particle first needs to be followed up to that event. Even though the deposited energy is used as an example here, what follows remains true for any variable that can be written in the form shown in equation 4.

The joint probability density function of the variables X_0 to X_n will here be written as

$$f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n}) \tag{5}$$

and the expected value of Y as

$$\mathbb{E}(Y) = \int_E h(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n}) f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n}) d\overrightarrow{x_0} d\overrightarrow{\omega}\, dx d\overrightarrow{x_n} \tag{6}$$

3. Conditional sampling of the scattering direction

Let us here assume that Y is a physical quantity computed in an area that particles have a very low probability of reaching. Then, estimations of properties of Y will potentially be very uncertain. This will show as a very high variance, and the estimations will require a large number of samples to be drawn. This can be somewhat improved by having more particles reaching the area of interest.

To reach the area of interest, the only way for a particle that is not directly emitted towards it is, first, to undergo a scattering event in which

it can be redirected towards it. If we define S as the set of directions that point towards the area of interest from the location of the interaction, then it would be helpful to sample, instead of $\overrightarrow{\Omega}$, the conditional variable giving the scattering direction *knowing* it is part of S, written as $\overrightarrow{\Omega}_{|\overrightarrow{\Omega}\in S}$, such that the particle will always be scattered in a direction with a high probability of contribution to the estimation.

However, this change of variable neglects the complementary set of directions, and the expected value of the new variable would be different from that of Y_n, thus biasing the estimation. To prevent this, one can first split the expected value of Y_n into two parts, by replacing Y_n with

$$Y_n \mathbb{1}_S(\overrightarrow{\Omega}) + Y_n \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}') \tag{7}$$

where $\mathbb{1}_S$ is the indicator function of the set S, $\mathbb{1}_{\overline{S}}$ is the indicator function of the complementary set $\overline{S}$, and both $\overrightarrow{\Omega}$ and $\overrightarrow{\Omega}'$ are defined by the same probability density function. It is clear that in this case, the expected value of the random variable in equation 7 is the same as that of Y_n.

Because we know that the expected value of $Y_n \mathbb{1}_S(\overrightarrow{\Omega})$ is

$$\mathbb{E}(g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})\mathbb{1}_S(\overrightarrow{\Omega})) = \int g(\overrightarrow{\omega}, x, \overrightarrow{x_n}) f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n}) \mathbb{1}_S(\overrightarrow{\omega}) d\overrightarrow{\omega}\, dx d\overrightarrow{x_n} \tag{8}$$

with

$$f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n})\mathbb{1}_S(\overrightarrow{\Omega}) = f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n} | \overrightarrow{\Omega} \in S) P(\overrightarrow{\Omega} \in S) \tag{9}$$

where $P(\overrightarrow{\Omega} \in S)$ denotes the probability that the direction $\overrightarrow{\Omega}$ is part of S, it is now possible to introduce the variable $\overrightarrow{\Omega}_{|\overrightarrow{\Omega}\in S}$ with no bias by replacing the sampling of $Y_n \mathbb{1}_S(\overrightarrow{\Omega})$ in equation 7 by that of the variable Y_s defined as

$$Y_s = g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})_{|\overrightarrow{\Omega}\in S} P(\overrightarrow{\Omega} \in S) \tag{10}$$

with the expected value

$$\mathbb{E}(Y_s) = \int g(\overrightarrow{\omega}, x, \overrightarrow{x_n}) f(\overrightarrow{x_0}, \overrightarrow{\omega}, x, \overrightarrow{x_n} | \overrightarrow{\Omega} \in S) P(\overrightarrow{\Omega} \in S) d\overrightarrow{\omega}\, dx d\overrightarrow{x_n} \tag{11}$$

which is, because of 9, equal to $\mathbb{E}(Y_n \mathbb{1}_S(\overrightarrow{\Omega}))$.

At this point, the sampling of the random variable Y_n has been replaced with

$$Y_n \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}') + Y_s \tag{12}$$

of same expected value. The sum indicates that two contributions need to be added, meaning that two particles now need to be followed. The first one is similar to Y_n, which is sampled by following a particle normally after the scattering event, but the indicator function shows that its contribution is non-zero only if its direction after the interaction is not part of S. In other words, the particle is killed if directed towards the area of interest after the scattering event. The second term is a particle which direction is sampled conditionally, knowing it is part of S, and will therefore always result in a particle scattered towards the area of interest. However, its contribution needs to be weighted by $P(\overrightarrow{\Omega} \in S)$.

4. Conditional sampling of the step

With the previous change of random variable, a particle is guaranteed to be directed towards the area of interest after the scattering event, but it might not be able to reach it without interacting again and will potentially be absorbed or scattered in another direction. The previous operation can be repeated for the distance travelled by the particle, this time by splitting the expected value of Y_s into two parts. If R is defined as the set of step values large enough for the particle to reach the area of interest and $\overline{R}$ as the complementary set, the random variable X now needs to be replaced with $X_{|X\in R,\overrightarrow{\Omega}=\overrightarrow{\omega}}$[1] to make sure a particle will reach the area of interest. As before, the variable Y_S is replaced by the sum of the two new variables :

$$Y_S \mathbb{1}_R(X)_{|\overrightarrow{\Omega}\in S} + Y_S \mathbb{1}_{\overline{R}}(X')_{|\overrightarrow{\Omega}\in S} \tag{13}$$

With X and X' following the same probability density function. Again, the expected value of the variable of equation 13 is equal to that of Y_S. In the same way as shown in part 3, the first term of this new variable can be replaced by the conditional variable

$$Y_{SR} = g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})_{|\overrightarrow{\Omega}\in S, X\in R} P(\overrightarrow{\Omega} \in S) P(X \in R | \overrightarrow{\Omega} = \overrightarrow{\omega}) \tag{14}$$

of same expected value. This new variable is the deterministic particle : its direction is sampled towards the area of interest, its step is large enough to

[1] Although it will not be written explicitly as $R(\Omega)$, it must be kept in mind that the set R depends on the value of Ω, hence the conditional dependance of X on $\Omega = \omega$.

reach it, but its contribution must be weighted by $P(\overrightarrow{\Omega} \in S)P(X \in R|\overrightarrow{\Omega} = \overrightarrow{\omega})$. Because the computation of $P(\overrightarrow{\Omega} \in S)$ can be very time-consuming, we can choose to replace $\overrightarrow{\Omega}_{|\overrightarrow{\Omega}\in S}$ with a random variable following a specifically chosen probability density function (also defined on S) using the importance sampling method (this is explained in MCNP's documentation [1]).

5. Handling of complementary particles

At this point, the expected value of the sampled random variable has been split twice into two parts and the expected value of Y_n is estimated by sampling three different variables, each corresponding to a particle that needs to be transported :

$$Y_{RS} + Y_S \mathbb{1}_{\overline{R}}(X')_{|\Omega\in S} + Y_n \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega'}) \tag{15}$$

However, the variable $Y_S \mathbb{1}_{\overline{R}}(X')_{|\Omega\in S}$, as written explicitly

$$g(\overrightarrow{\Omega}, X', \overrightarrow{X_n})_{|\overrightarrow{\Omega}\in S} P(\overrightarrow{\Omega} \in S)\mathbb{1}_{\overline{R}}(X')_{|\overrightarrow{\Omega}\in S} \tag{16}$$

can be replaced with the variable of same expected value (see property 9) :

$$g(\overrightarrow{\Omega}, X', \overrightarrow{X_n})\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(X') \tag{17}$$

which can also be written as

$$Y_n \mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(X') \tag{18}$$

The sampled variable then becomes

$$Y_{RS} + Y_n \mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(X') + Y_n \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega'}) \tag{19}$$

Finally, the last two terms of the random variable in equation 19 can then be merged with no change to the expected value to create the random variable associated to pseudo-deterministic transport :

$$Y_{RS} + Y_n \left[\mathbb{1}_S(\overrightarrow{\Omega'})\mathbb{1}_{\overline{R}}(X') + \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega'})\right] \tag{20}$$

with, again, $\overrightarrow{\Omega'}$ defined by the same probability density function as $\overrightarrow{\Omega}$. The second variable of equation 20 can be sampled by following only one particle

instead of two as in equation 15, thus saving computer time. This particle is transported in a completely analog manner, except that its contribution to any estimation will only be non-zero at the condition that it is either not directed towards the area of interest, or it is directed towards it but doesn't reach it within its next step. In other words, the particle must be killed if it enters the area of interest in the step following the interaction. This complementary particle is similar to the "non-deterministic" particle from the DXTRAN method. As each step retained the expected value of the previous sampled variable, it can be shown that

$$\mathbb{E}\left(Y_{RS} + Y_n\left[\mathbb{1}_S(\overrightarrow{\Omega'})\mathbb{1}_{\overline{R}}(X') + \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega'})\right]\right) = \mathbb{E}(Y_n) \tag{21}$$

6. Handling of secondary particles produced

In the final expression of the random variable associated with pseudo-deterministic transport in equation 20, both $g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})_{|\overrightarrow{\Omega}\in S}$ and $g(\overrightarrow{\Omega}', X', \overrightarrow{X_n}')$ appear when explicitly writing Y_{RS} and Y_n. Those functions depend on $\overrightarrow{X_n}$ or $\overrightarrow{X_n}'$, which are themselves sampled by transporting the scattered particle after the interaction where pseudo-deterministic transport was applied. This includes any secondary particles produced, such as the recoil electron from a Compton scattering, whose energy depends on $\overrightarrow{\Omega}$.

Taking Compton scattering as an example, this means two recoil electrons with different energy need to be transported : one associated to the deterministic photon and carrying the same weight, and one associated to the complementary photon and which must be killed if the photon enters the area of interest. This would cause a substantial increase in computation time, but can be avoided by transporting only the recoil electron produced by the complementary photon, with no weight or kill condition. This also applies to any secondary particle produced, such as X-ray emitted by the atomic relaxation after being ionised by the scattering interaction.

Let us write as $\overrightarrow{X_p}$ every random process encountered by the primary particle, and as $\overrightarrow{X_s}$ every random process encountered by any secondary particle produced by the scattering interaction. Then the variable Y_n (see equation 4) can also be written as :

$$Y_n = g(\overrightarrow{\Omega}, \overrightarrow{X_p}, \overrightarrow{X_s}) \tag{22}$$

Assuming the energy deposited by the entire particle track is being scored, then the function g is the sum of the contributions of the primary particle and of the secondary particles and can be written as :

$$Y_n = g(\overrightarrow{\Omega}, \overrightarrow{X_p}, \overrightarrow{X_s}) = h(\overrightarrow{\Omega}, \overrightarrow{X_p}) + h'(\overrightarrow{\Omega}, \overrightarrow{X_s}) \tag{23}$$

Notice that in this case, the scattering angle $\overrightarrow{\Omega}$ is sampled as the interaction takes place, and both the next processes of the primary and of the secondary particles produced depend on its value. That is why applying pseudo-deterministic transport, as shown in section 3, by first splitting $\overrightarrow{\Omega}$ according to whether or not the particle is directed towards the area of interest would create two sets of primary and two sets of secondary particles to be simulated.

However, if we introduce the variable $\overrightarrow{\Omega}'$ of same probability density function as $\overrightarrow{\Omega}$, then we have

$$\mathbb{E}\left(Y_n\right) = \mathbb{E}\left(h(\overrightarrow{\Omega}, \overrightarrow{X_p}) + h'(\overrightarrow{\Omega}', \overrightarrow{X_s})\right) \tag{24}$$

In this step, the scattering angle associated to the secondary particles is independent from $\overrightarrow{\Omega}$ and must be sampled separately.

Then, in order to apply pseudo-deterministic transport, one first needs to split the random variable according to the scattering angle of the primary photon as shown in section 3. The variable $h(\overrightarrow{\Omega}, \overrightarrow{X_p})$ in equation 23 is then replaced by :

$$h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega}) + h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}) \tag{25}$$

As before, it can be shown that

$$\mathbb{E}(Y_n) = \mathbb{E}\left(h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega}) + h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}) + h'(\overrightarrow{\Omega}', \overrightarrow{X_s})\right) \tag{26}$$

Then, the variable $h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega})$ is split according the the distance travelled during the next step, and becomes

$$h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_R(\overrightarrow{\Omega}) + h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(\overrightarrow{\Omega}) \tag{27}$$

We now have :

$$\begin{aligned}\mathbb{E}(Y_n) = \mathbb{E}\Big(& h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_R(\overrightarrow{\Omega}) + h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(\overrightarrow{\Omega}) \\ & + h(\overrightarrow{\Omega}, \overrightarrow{X_p})\mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}) + h'(\overrightarrow{\Omega}', \overrightarrow{X_s})\Big)\end{aligned} \tag{28}$$

The variable $\overrightarrow{\Omega}$ can now be replaced with $\overrightarrow{\Omega}'$ and $\overrightarrow{X_p}$ with $\overrightarrow{X_p}'$ of same probability density function in the second and third terms (associated with the complementary particles) of equation 28 such that we can write

$$\begin{aligned}\mathbb{E}(Y_n) = \mathbb{E}\Bigg(& h(\overrightarrow{\Omega}, \overrightarrow{X_p}) \mathbb{1}_S(\overrightarrow{\Omega}) \mathbb{1}_R(\overrightarrow{\Omega}) \\ & + h(\overrightarrow{\Omega}', \overrightarrow{X_p}') \left[\mathbb{1}_S(\overrightarrow{\Omega}') \mathbb{1}_{\overline{R}}(\overrightarrow{\Omega}') + \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega}') \right] \\ & + h'(\overrightarrow{\Omega}', \overrightarrow{X_s}) \Bigg)\end{aligned} \tag{29}$$

In the first term inside the expected value of equation 29, $\overrightarrow{\Omega}$ and $\overrightarrow{X_p}$ can be replaced with the weighted conditional variables $\overrightarrow{\Omega}_{|\overrightarrow{\Omega} \in S} P(\overrightarrow{\Omega} \in S)$ and $\overrightarrow{X_p}_{|\overrightarrow{X_p} \in R} P(\overrightarrow{X_p} \in R)$ as was done in parts 3 and 4 in order to formulate the expected value of a random variable representing a deterministic particle as shown in equation 14. The next term is the expression of the complementary particle, as in the second term of equation 20, and the last one represents the secondary particles produced by the interaction, which, in this case, are not impacted by replacing the scattering angle $\overrightarrow{\Omega}$ with a conditional variable.

Notice that last two variables in the expected value of equation 29 are sampled by drawing only one scattering angle $\overrightarrow{\Omega}'$, and then transporting the associated primary particle ($\overrightarrow{X_p}'$) and only one set of secondary particles ($\overrightarrow{X_s}$). Taking the example of a Compton scattering, this means the recoil electron's energy and direction are those associated to the complementary photon's scattering angle.

7. Use with specific estimators

Up to this point, it was assumed that a sample of the studied random variable was the sum of contributions from all the particles involved in the track of a source particle, such as the deposited energy per source particle which includes not only the energy deposited by both the deterministic particle and the complementary particle, but also the secondary particles produced. However, it is not the case for all possible estimations and the use of pseudo-deterministic transport might require changes in how quantities are scored compared to a simulation with no variance reduction.

In the case of a pulse height estimator on an energy interval B_i, the random variable takes for value 1 if the energy deposited during the particle

track falls into the interval B_i and 0 otherwise. The sampled variable can therefore be written as

$$Y^{pulse} = \mathbb{1}_{B_i}(E) \tag{30}$$

Where E is the energy deposited during the particle track. This deposited energy is itself a function of every physical process taking place during the particle track, such that Y^{pulse} can be written

$$Y^{pulse} = h^{pulse}(\overrightarrow{X_0}, \overrightarrow{\Omega}, X, \overrightarrow{X_n}) \tag{31}$$

as was done in equation 3. In this case however, Y^{pulse} usually cannot be written as the sum of the two contributions before and after the scattering event where pseudo-deterministic transport is used. In a simulation without variance reduction, the total energy deposited by all particles in the track would be computed and then checked against B_i to determine the value of Y^{pulse}, which could be written as

$$h^{pulse}(\overrightarrow{X_0}, \overrightarrow{\Omega}, X, \overrightarrow{X_n}) = \mathbb{1}_{B_i}(g_0(\overrightarrow{X_0}) + g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})) \tag{32}$$

where $g_0(\overrightarrow{X_0})$ and $g(\overrightarrow{\Omega}, X, \overrightarrow{X_n})$ are the energies deposited before and after the scattering event. Instead of being the sum of both contributions, Y_{pulse} is a function of this sum. Assuming the way the energy is scored is not changed when using pseudo-deterministic transport, the pulse height estimations would be biased as condition 4 is not met. As it cannot be expressed as a sum, applying pseudo-deterministic transport without first separating the contributions would yield :

$$\begin{aligned} &h^{pulse}_{pseudo-det}(\overrightarrow{X_0}, \overrightarrow{\Omega}, X, \overrightarrow{X_n}) \\ &= h^{pulse}(\overrightarrow{X_0}, \overrightarrow{\Omega}, X, \overrightarrow{X_n})_{|X\in R, \overrightarrow{\Omega}\in S} P(\overrightarrow{\Omega} \in S) P(X \in R | \overrightarrow{\Omega} = \overrightarrow{\omega}) \\ &\quad + h^{pulse}(\overrightarrow{X_0}, \overrightarrow{\Omega}', X', \overrightarrow{X_n}')[\mathbb{1}_S(\overrightarrow{\Omega})\mathbb{1}_{\overline{R}}(X) + \mathbb{1}_{\overline{S}}(\overrightarrow{\Omega})] \end{aligned} \tag{33}$$

where $\overrightarrow{\Omega}'$, X' and $\overrightarrow{X_n}'$ respectively follow the same probability density function as $\overrightarrow{\Omega}$, X and $\overrightarrow{X_n}$.

Contrary to what was previously done, the contribution of the entire track that contains the deterministic particle now needs to be weighted, while the entire contribution from the track of the complementary particle will be set to zero if it enters the area of interest during its next step.

Some considerations about the secondary particles produced by the interaction also need to be made for pulse height estimations : in the previous

section, the contributions to the estimation from the two sets of secondary particles produced by the application of pseudo-deterministic transport were merged into a single set of particles because the expected value of the random variable could be written as the sum of both contributions. However, in this case, using notations defined in section 6, it can be written as :

$$g^{pulse}(\overrightarrow{X_0}, \overrightarrow{\Omega}, \overrightarrow{X_p}, \overrightarrow{X_s}) = \mathbb{1}_{B_i}\big(h_0(\overrightarrow{X_0}) + h(\overrightarrow{\Omega}, \overrightarrow{X_p}) + h'(\overrightarrow{\Omega}, \overrightarrow{X_s})\big) \tag{34}$$

In this case, the total energy deposited by the source particle is computed by summing the energy deposited before, during and after the scattering event. Then, the contribution of the source particle is 1 if the total energy falls into the interval B_i and zero otherwise. We can see that in this case the random variable is not a sum of the three contributions but again a function of this sum. This means the process devised in 6 cannot be applied to merge the two sets of secondary particles into a single one and both need to be transported.

Finally, in the case of an energy spectrum estimation, which consists of obtaining the distribution of the energy of particles entering a specific region, multiple energy intervals are defined and each corresponds to a unique random variable. In each particle track, the number of particles with an energy contained in each interval is tallied. This means contributions from all particles are scored independently and the sampled variable for a given interval B_i, can be written as :

$$Y^{spectrum} = \sum_{j=1}^{N} \mathbb{1}_{B_i}(E_j) \tag{35}$$

where E_j is the energy of the j^{th} entering particle. With E_1 to E_{k-1} the energy of particles entering before the scattering event and E_k to E_N the energy of particles entering after, $Y^{spectrum}$ can be written as :

$$Y^{spectrum} = \sum_{j=1}^{k-1} \mathbb{1}_{B_i}(E_j) + \sum_{j=k}^{N} \mathbb{1}_{B_i}(E_j) \tag{36}$$

which can be expressed as a sum of functions g_0 and g_n of the energy of entering particles :

$$Y^{spectrum} = g_0^{spectrum}(E_1 \dots E_{k-1}) + g_n^{spectrum}(E_k \dots E_N) \tag{37}$$

The energy of particles 1 to $k-1$ are functions of every random process occuring before the scattering event, $\overrightarrow{X_0}$, and similarly, the energy of particles

k to N are functions of processes $\overrightarrow{\Omega}$, X and $\overrightarrow{X_n}$. As such, $Y^{spectrum}$ can also be written as :

$$Y^{spectrum} = h_0^{spectrum}(\overrightarrow{X_0}) + h_n^{spectrum}(\overrightarrow{\Omega}, X, \overrightarrow{X_n}) \tag{38}$$

This allows for the use of pseudo-deterministic transport (applied to the second term of equation 38) without any change to scoring.

In the case of energy spectrum estimations, the sampled random variable can also be written as the sum of contributions from the primary particle and secondary particles produced by the scattering event in the same way as the deposited energy, and the two sets of secondary particles produced by the pseudo-deterministic transport can be merged into a single one.

8. Conclusion

Among the many available variance reduction techniques, pseudo-deterministic transport seems to be one of the most promising for improving the sampling of a region in space that particles have trouble reaching, by forcing particles to reach an arbitrarily chosen region (usually spherical).

We have shown that this method can be applied to any scattering event during the transport of a particle, by splitting the particle track twice depending first on the scattering direction and then on the distance travelled before interacting again. Among the three particles created, one is a weighted "deterministic" particle, allowed to reach the desired area by conditionally sampling the scattering direction and the travelled distance. The other two can be regrouped without bias into a single particle carrying no weight modification, but that must be killed if it enters the area of interest during its next step.

We have also shown that secondary particles created by the scattering event can, when the sampled variable can be expressed as the sum of every particle's contribution, be merged into a single set of secondary particles associated with the complementary particle of the pseudo-deterministic transport while keeping the expected value of the original variable.

Finally, some considerations were made about which estimators can be used with this method and how this might impact how simulation codes tally the quantities of interest. Pseudo-deterministic transport can be used with energy spectrum estimators without any change to scoring, but it will bias pulse height estimators assuming the code tallies the total energy deposited

during the particle track with no regard to which type of particle interacted (deterministic or complementary). Merging the two sets of secondary particles created by the scattering event also does not work with pulse height estimators, and both need to be transported.

This works provides a basis for an unbiased implementation of the pseudo-deterministic transport method in a Monte Carlo simulation transport code, which can be used to solve problems related to the under-sampling of a specific region in space.

Declaration of competing interest

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References

[1] X-5 Monte Carlo Team, MCNP - A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory, LA-UR-03-1987, Los Alamos National Laboratory, 2003.