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FEASIBILITY OF AN ADJOINT MONTE CARLO PULSE HEIGHT SPECTRUM CALCULATION

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ABSTRACT

The usefulness of adjoint Monte Carlo calculations has been recognized decades ago. An adjoint Monte Carlo game can only be played, if sufficient formulation of responses can be made. For quantities that cannot be described by the integral Boltzmann equation, a formulation in the conventional way is not possible. This paper describes a scheme for the adjoint sampling of a non-Boltzmann tally, the distribution of total energy release by a particle in the detector in a non-multiplying system.

Key Words: Monte Carlo, adjoint, pulse height spectrum, non-Boltzmann tally

1. INTRODUCTION

Monte Carlo calculations of radiation transport problems can be considered as direct simulation of processes occurring in nature (heuristic interpretation) or as a solution to the integral form of the Boltzman transport equation. An important feature of the heuristic interpretation is that quantities can be estimated that can not be described solely by the solution of the Boltzmann equation (non-Boltzmann tallies). For normal Boltzmann tallies, in practice, instead of an analogue simulation where samples represent possible trajectories of real particles, a biased game is played, where a statistical analogue of the former is realized due to efficiency reasons. Verification for such biases can be obtained using heuristic reasoning to a certain extent [5,6], but can be more easily obtained from manipulation of the integral formulation. Considering the non-Boltzmann tallies, the integral formulation was extended [3] resulting in the so-called score probability equations. These extensions, however, did not include formulations for all possible quantities of interest, resulting in codes and methods where analogue (unbiased) Monte Carlo simulation is recommended and the use of non-analogue simulation instead, is passionately debated.

In most cases, biasing of the Monte Carlo simulation for higher efficiency is possible because of the absence of combined effects of multiple particles. For exact simulation of measurements these criteria can fail [1], and speed-up techniques must be separately investigated [7]. A useful statistical analogue is the adjoint Monte Carlo simulation, originating from the adjoint form of the integral Boltzmann equation. In an adjoint simulation, particles are started from the detector instead of the source, and they score in the source domain instead of the detector. This method has already been investigated as a method to calculate integrals of the adjoint flux (adjoint

function) [2]. A special case occurs, when the adjoint flux is integrated over the source function. This then this yields the detector response as it is stated by the general reciprocity theorem. The adjoint function is not defined when estimating non-Boltzmann tallies. However, an adjoint (reversed) Monte Carlo solution for the detector response is possible. In this paper a method of estimating a non-Boltzmann tally (the distribution of total energy release by a particle in the detector) by adjoint Monte Carlo is presented.

2. FORWARD AND ADJOINT MONTE CARLO

The integral equation formalism behind transport Monte Carlo is based on the following form:

$$y\ (P) = S(P) + \int K\left(P' \to P\right) y\ (P')\, dP' \tag{1}$$

The response can be described as:

$$R = \int h(P)\, y\ (P)\, dP \tag{2}$$

Here P is the phase-space variable, $S(P)$ is the source function, $h(P)$ the detector response function, $K\left(P' \to P\right) dP$ is the probability that a particle has coordinate P in dP at a collision if its previous collision was at P', and $y\ (P)$ represents the number of particles at a collision. Depending on the actual definition of $K\left(P' \to P\right)$, $y\ (P)$ is interpreted as the number of particles emitted with coordinate P after a collision or entering a collision.

The equation adjoint to Eq.(1) is

$$y^{+}\left(P\right) = h(P) + \int K\left(P \to P'\right) y^{+}\left(P'\right) dP' \tag{3}$$

and a response is to be found in the form of

$$R^{+} = \int y^{+}\left(P\right) g\left(P\right) dP \tag{4}$$

The reciprocity theorem states that if $g(P) = S(P)$ then $R = R^{+}$.

When simulating the first equation, samples are selected from the source and, by repeated sampling of the kernel K, subsequent co-ordinates are chosen. When solving the adjoint equation initial co-ordinates are selected according to the scoring function of the forward formulation and new co-ordinates are determined using the same K kernel, but with P and P' interchanged.

The Monte Carlo sampling of such integral equations will be briefly summarized. Integrals of functions can be calculated by the Monte Carlo method. To arrive at the solution of integrals of

functions defined by an integral equation, we may consider the following: let $y_1(P)$ be an unknown probability density function (pdf), $y_0(P)$ a known pdf, $K(P' \to P)$ a nonnegative function, and let

$$y_1(P) = \int K(P' \to P) y_0(P') dP' \tag{5}$$

The aim is to determine the integral

$$I_1 = \int h(P) y_1(P) dP \tag{6}$$

using an arbitrary function $h(P)$. This problem can be solved by Monte Carlo, by defining the conditional pdf

$$k(P \mid P') = \frac{K(P' \to P)}{\int K(P' \to P'') dP''} \tag{7}$$

and selecting P' from $y_0(P')$, selecting P according to the conditional pdf $k(P|P')$ and calculating

$$I_1 = \mathcal{E}\left[\frac{1}{N} \sum_{i=1}^{N} h(P_i) . \int K(P_i \to P'') dP'' \right] \tag{8}$$

If $y(P)$ of Eq.(1) can be written as a sum of functions that are connected recursively like those in Eq. (5), then the response R of Eq.(2) can also be expressed as a sum of integrals like the one shown in Eq.(6).
If we wish to reverse the process and draw samples from the scoring function $h(P)$, the feasibility of such a game can be proven. A simple "adjoint" (reversed) method for calculating the same integral can be formulated from the previous equations. If we put the expression for $y_1(P)$ into the expression for I_1, we get

$$I_1 = \int h(P) \int K(P' \to P) y_0(P') dP' dP = \int y_0(P) \int h(P') K(P \to P') dP' dP \tag{9}$$

If $h(P)$ is a nonnegative function, selecting P' from $h(P')/\int h(P'')dP''$, and P from

$$k^+(P \mid P') = \frac{K(P \to P')}{\int K(P'' \to P') dP''}, \tag{10}$$

the final expression can be estimated as

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} y_0(P_i).\int K(P' \to P_i)dP'.\int h(P'')dP'' \tag{11}$$

since the expected value of this expression is

$$\begin{aligned} &\mathcal{E}\left[\hat{I}\right] = \mathcal{E}\left[\frac{1}{N}\sum_{i=1}^{N} y_0(P_i).\int K(P' \to P_i)dP'.\int h(P'')dP''\right] = \\ &= \int\int h(P'')\,k^{+}(P''|P')y_0(P')\int K(P \to P')dP'dPdP'' = \int h(P)y_1(P)dP \end{aligned} \tag{12}$$

In the forward case, when a chain of functions is constructed by repeated application of Eq.(5),

$$y_j(P) = \int K(P' \to P)y_{j-1}(P')dP', \tag{13}$$

with the first (source) function known, the integral

$$I_j = \int h(P)y_j(P)dP \tag{14}$$

can be estimated by Monte Carlo for any j in the following way. First select an initial co-ordinate P_0 from the first function of the chain $y_0(P)$, select the next co-ordinate P_1 from

$$k(P \mid P_0) = \frac{K(P_0 \to P)}{\int K(P_0 \to P')dP'} \tag{15}$$

and set a weight factor to $w_0 = \int K(P_0 \to P')dP'$. After this, keep repeating the process of selecting P_i from $k(P_i|P_{i-1})$ and of setting $w_i = \int K(P_{i-1} \to P')dP$ until j is reached. Then a sample of the estimator for I_j is obtained:

$$\hat{I}_j = h(P_j)\prod_{i=0}^{j-1} w(P_i) \tag{16}$$

and an average of these samples is the final estimate of I_j. The proof for this can be found in reference [4]. It can be also shown that a solution for an integral $R = \int h(P)y(P)dP$ with $y(P)$ defined by an integral equation like Eq.(1) is given by the sum

$$R = \sum_{j=0}^{\infty} I_j \tag{17}$$

The integral I_j can be estimated by adjoint Monte Carlo as well by changing the order of integrations in the chain of recursive functions like in Eq.(9):

$$I_j = \int h(P_j) \int K(P_{j-1} \to P_j) \ldots \int K(P_0 \to P_1) S(P_0)\, dP_0 \ldots dP_j = \\ = \int S(P_j) \int h(P_0) K(P_1 \to P_0) \ldots \int K(P_j \to P_{j-1}) dP_0 \ldots dP_j. \tag{18}$$

If a sample is selected from the detector function $h(P)$, and the next samples are drawn from the kernel k^+ of Eq.(10), then, if setting the adjoint weight factor to $w^+ = \int K(P \to P_{i-1})\, dP$, an adjoint sample for I_j can be obtained as

$$\hat{I}_j = S(P_j) \prod_{i=0}^{j-1} w^+(P_i) \tag{19}$$

Such a form is often derived from the adjoint equation (3) following the derivation for the forward Monte Carlo solution. With this line of thought, however, we can arrive at a derivation that does not need the statement of the adjoint equation, but verifies the adjoint Monte Carlo process with results coincident with the solution to the adjoint transport equation.

3 INTEGRATION WITH CONSTRAINTS

Time independent particle transport simulations can also be described by a single pdf that is a function of the coordinates of all collisions. This pdf consists of a multiplication of conditional pdf's $\wp(P_i \mid P_{i-1})$, expressing the probability of a particle reaching a phase space coordinate P_i if the previous collision happened at P_{i-1}. Usually we want to estimate an expected value, which can be expressed as:

$$\mathcal{E}[h(P_0, P_1, \ldots, P_n)] = \int \ldots \int h(P_0, P_1, \ldots, P_n) \prod_{i=1}^{n} \wp(P_i \mid P_{i-1}) dP_n \ldots dP_0 \tag{20}$$

In certain cases this may have to be specified further: the scoring function dependent on the phase space coordinates may also depend on the actual process leading to P_i (absorption, free flight, scattering). Then the pdf must be broken up into other pdf's defining, for example, the pdf of traveling from one collision point to another and the pdf of post-collision coordinates assuming the pre-collision ones. Often the scoring function h can be transformed into simpler forms when it depends on one phase-space point, rather than on multiple collisions together. In those cases a corresponding score equations can be formulated, or it can be well represented by a partially biased estimator. In the most general case the response can be dependent on several independent chains like in reactor noise measurement simulations [1], where a different statistical model needs to be set up. However, now we will restrict ourselves to handling non-multiplying single chains.

An important irreducible chain is when h is setting a constraint for the integration, which constraint depends on the indexed collision points P_i.

With the commonly used notations we might formulate an integral that is aimed to be solved by neutral particle transport Monte Carlo of the following form:

$$I = \int ... \int S(P_0) \prod_{i=1}^{\infty} K(P_{i-1} \rightarrow P_i) h(P_1, ..., P_\infty) dP_\infty ... dP_0, \tag{21}$$

where the scoring function h can be split up into a function defining the domain of the integration and a function that accounts for the magnitude of the score. Calculating such an integral by forward Monte Carlo includes sampling from the source function, selecting the next coordinates from the transport kernel, and scoring according to the scoring functions. In an adjoint mode the particles should start from the termination probability in the system, and their travel should be followed (sampling the kernel *K* backwards) and their contribution to be tallied in the scoring functions.

Later on we will investigate an equivalent form where the integral is defined like:

$$I = \sum_{n=1}^{\infty} \int ... \int S(P_0) \prod_{i=1}^{n-1} K_s(P_{i-1} \rightarrow P_i) K_a(P_{n-1} \rightarrow P_n) h_n(P_0, ..., P_n) dP_n ... dP_0, \tag{22}$$

where $K_a(P \rightarrow P')$ is the transport kernel where the collision results in an absorption

$$K_a(P \rightarrow P') = T(r \rightarrow r' | E, \Omega) \frac{\Sigma_a(r', E)}{\Sigma_t(r', E)} d(E') d(\Omega' - \Omega_a) \tag{23}$$

with W_a an arbitrary direction, and $K_S(P \rightarrow P')$ is the transport kernel where the collision results in a scattering

$$K_s(P \rightarrow P') = T(r \rightarrow r' | E, \Omega) \frac{\Sigma_s(r', E \rightarrow E', \Omega \rightarrow \Omega')}{\Sigma_t(r', E)}. \tag{24}$$

$h_n(P_0,\ldots,P_n)$ is a characteristic function equal to 1 for those parts of the phase space describing the domain of integration including the source function, but zero elsewhere.
It might be made more sophisticated by distinguishing between pay-offs of different parts of the joint kernel, e.g. the track length estimator is a pay-off that gives a contribution according to the displacement kernel *T* only.

3.1. The Constraint for the Flux

When simple scoring functions are used, an integral equation can be derived to which the chain is a solution. When calculating the particle flux, the estimator is dependent only on the particle's phase-space coordinate. For such an estimator as the flux is, the scoring function h will be chosen according to

$$h(P_0, ..., P_\infty) = S(P_0) \sum_{j=1}^{\infty} h(P_j) \tag{25}$$

When we substitute this into Eq.(20) we can write:

$$I = \int ... \int S(P_0) \sum_{j=1}^{\infty} h\left(P_j\right) \prod_{i=1}^{\infty} K\left(P_{i-1} \to P_i\right) dP_\infty ... dP_0 =$$
$$= \sum_{j=1}^{\infty} \left\{ \int ... \int S(P_0) h\left(P_j\right) \prod_{i=1}^{j} K\left(P_{i-1} \to P_i\right) \prod_{i=j+1}^{\infty} K\left(P_{i-1} \to P_i\right) dP_\infty ... dP_0 \right\}. \tag{26}$$

Next, we define the function

$$y_j\left(P_j\right) = \int ... \int S(P_0) \prod_{k=1}^{j} K(P_{k-1} \to P_k) dP_{j-1} .. dP_0 \qquad j = 1,2,... \tag{27}$$

to get

$$I = \sum_{j=1}^{\infty} \int y_j(P_j) h(P_j) \left\{ \int ... \int \prod_{i=j+1}^{\infty} K(P_{i-1} \to P_i) dP_\infty ... dP_{j+1} \right\} dP_j \tag{28}$$

The joint kernel K is usually normalized to unity for the outgoing coordinates in an infinite medium. Therefore $\int\int K\left(P_1 \to P_2\right) K\left(P_2 \to P_3\right) dP_2 dP_3 = \int K\left(P_1 \to P_2\right) dP_2 = 1$. From this we can conclude that the part in braces of Eq.(27) is unity, as $\int ... \int \prod_{i=j+1}^{n} K\left(P_{k-1} \to P_k\right) dP_\infty ... dP_{j+1} = 1$ for arbitrary n .The integral takes a form of

$$I = \sum_{j=1}^{\infty} \int y_j(P_j) h(P_j) dP_j \tag{29}$$

This form is the same as Eq.(13) and Eq.(16) combined, and the definition in Eq.(26) is equivalent to the application of Eq.(5) for higher indices. Such an integral can be solved by adjoint Monte Carlo as well, as stated earlier. Taking Eq.(28) and the same number of scattering collisions n. We can change the numbering of n going backward from n to zero. Moreover, let us set

$$I = \sum_{j=1}^{n} \int y_j(P_j) h(P_j) dP_j =$$
$$\sum_{j=1}^{n} \int ... \int S(P_0) h\left(P_j\right) \prod_{i=1}^{j} K(P_{i-1} \to P_i) dP_j ... dP_0 = \tag{30}$$
$$\sum_{l=1}^{n} \int ... \int S(P_l) h\left(P_0\right) \prod_{i=1}^{l} K(P_i \to P_{i-1}) dP_l ... dP_0$$

The last expression gives the adjoint scheme, with samples taken from the scoring function $h(P_0)$ (usually only non-zero in the detector domain), and sample successive coordinates from the kernel K with variables interchanged. The scoring is made by the source function S, and the contributions of a particle should be summed.

3.2. Distribution of Energy Release in the Detector

A simple non-Boltzmann quantity that is frequently simulated is the probability distribution of the total energy release of a particle in a space-domain. Such a problem can originate from time-dependent detector responses, e.g. when the detector's time resolution of pulses is larger than the average lifetime of a particle, though stays in the same order magnitude. Heuristically, calculating such a quantity is not a problem for a Monte Carlo code, though usage of variance reduction can be debated: e.g. if a particle trajectory is split in the detector only a heuristic reasoning could be given for verification.
A much bigger problem is the possibility of adjoint sampling of the detector, if -for efficiency or other reasons- it seems advantageous to be used.
The constraint for the energy release probability could be formulated regarding n-long scattering chains ending with absorption, like in Eq.(21). The kernels determine the energy release, noted as $DE_i=E_{i-1}-E_i$. The phase space coordinate determines whether the collision happened in the detector. We will use the symbol $\Pi_{E_d,\Delta E_d}(E)$ for the function that is zero if E is not in within the interval $[E_d,E_d+DE_d]$ and 1 otherwise. $\Pi_{\mathbf{r}\in V_d}(\mathbf{r})$ is zero if $\mathbf{r}$ is not in the detector domain, 1 otherwise. With these notations the constraint for total energy release in the detector for an n-long chain will look like:

$$h\left(P_0,\ldots,P_n\right)=\Pi_{E_d,\Delta E_d}\left(\sum_{i=1}^{n}\Delta E_i\,\Pi_{\mathbf{r}\in V_d}\left(\mathbf{r}_i\right)\right) \tag{31}$$

We can insert this into Eq.(21)

$$I=\sum_{n=1}^{\infty}\int\ldots\int K_a\left(P_{n-1}\to P_n\right)S\left(P_0\right)\Pi_{E_d,\Delta E_d}\left(\sum_{i=1}^{n}\Delta E_i\,\Pi_{\mathbf{r}\in V_d}\left(\mathbf{r}_i\right)\right)\prod_{j=1}^{n-1}K_s\left(P_{j-1}\to P_j\right)dP_n\ldots dP_0. \tag{32}$$

Satisfying such a constraint is not troublesome in the forward game, especially if a full, detailed spectrum is to be estimated. However, it becomes harder to bias the game for higher efficiency if only a certain part of the spectrum is important, or to play an adjoint game. The latter difficulty does not lie in the sampling of the kernels or satisfying the energy constraint, but in sampling it efficiently. According to this response function, samples should be drawn from the entire geometry from the energy distribution of absorption, and if crossings are made through the detector and the source, in both cases should "score"(or more frequently samples should be omitted). A possible geometrical restriction to the detector volume in the adjoint sampling may be considered: it is feasible to start an adjoint sample from the detector volume, and check if it reaches the detector. To obtain the total deposited energy, we can start from the same point (but in the opposite direction) a forward particle, to "finish" the history. In this article we will focus on the possibility of a fully adjoint solution.

To derive a suitable form for sampling, we need to break up the response function to sums of terms where the integration specifies the space-domain of the detector. As the spatial constraint is dependent on the domain of the detector, it seems possible to draw samples from only the detector region, making the adjoint calculation's aims feasible, namely to decouple the calculation to a detector function dependent on the flux or to transport particles, when a, from calculational point of view, source and detector space-domains are interchanged.

The last collision of the particle will either be in the detector volume and its energy will contribute to the sum of deposited energies, or will be out of the detector volume and its energy is irrelevant for the detector-reading. It can be expressed as:

$$
\begin{aligned}
&h\left(P_0,\ldots,P_n\right)=\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n}\Delta E_i\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)= \\
&\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_n\right)\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)+\Delta E_n^{a}\right)+\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)\left(1-\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_n\right)\right)= \\
&=\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_n\right)\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)+\Delta E_n^{a}\right)-\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_n\right)+ \\
&+\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)
\end{aligned}
\tag{33}
$$

where the superscripts *a* and *s* are distinguishing the energy release of an absorption from a scattering event respectively. The first two terms of the three we obtained in Eq.(33) express the sampling of a point from the detector volume. The third term is a sampling from a point outside the detector region. The third term cannot be sampled thus from the detector domain, and needs to be expressed by other terms. Decomposing it in the same way as above (Eq.33):

$$
\begin{aligned}
&\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)= \\
&\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_{n-1}\right)\left\{\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-2}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)+\Delta E_{n-1}^{s}\right)-\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-2}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right)\right\} \\
&+\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-2}\Delta E_i^{\,s}\prod_{\boldsymbol{r}\in V_d}\left(\boldsymbol{r}_i\right)\right).
\end{aligned}
\tag{34}
$$

The last term can be decomposed, yielding a term the same as Eq.(33) with the indices reduced by one. This process can be repeated yielding recursion, leading to the following form of the response function:

$$h(P_0,...,P_n)=\prod_{\mathbf{r}\in V_d}(\mathbf{r}_n)\left\{\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)+\Delta E_n^{a}\right)-\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{n-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)\right)\right\}$$
$$+\sum_{k=1}^{n-1}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_k)\left\{\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{k-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)+\Delta E_k^{s}\right)-\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{k-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)\right)\right\} \quad (35)$$

The term in the second line is still not suitable for the adjoint sampling as it contains terms, when samples for r_n should be taken from the whole model volume, from the absorption probability. Putting this form (second term of Eq.(35)) into the transport integral of Eq.(21), and changing the order of integrations and the summation over *n*, we obtain the following:

$$\sum_{n=1}^{\infty}\int...\int S(P_0)K_a(P_{n-1}\to P_n)\times$$
$$\times\sum_{k=1}^{n-1}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_k)\left\{\prod_{E_d,\Delta E_d}\left(\sum_{i=1}^{k-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)+\Delta E_k^{s}\right)-\prod_{E_d,\Delta E}\left(\sum_{i=1}^{k-1}\Delta E_i^{\,s}\prod_{\mathbf{r}\in V_d}(\mathbf{r}_i)\right)\right\} \quad (36)$$
$$\times\prod_{i=1}^{n-1}K_s(P_{i-1}\to P_i)\,dP_n...dP_0.$$

The summation over *n* is a summation of all possible lengths of chains, the index *k* expresses the number of collisions until the last event in the detector. The last event in the detector (the k^{th}) is followed by *n-k* collisions that will not contribute to the response estimator independently of their exact phase-space positions as long as they are outside the detector. For our purpose it is more convenient to change the order of the summations, selecting the ordinal numeral of the last event in the detector (*k*) multiplied by the sum of terms expressing the lengths of the chains from *k* to infinity, and also multiplied by the corresponding scattering and absorption kernels. To avoid very lengthy formulation, and to show the index changes in a simplified form, we select s_0 for the source expression, a_k for the response functions, and b_i for the kernel terms using *i* for the outgoing coordinates. Omitting the integrations we obtain:

$$s_0\sum_{n=1}^{\infty}\sum_{k=1}^{n-1}\prod_{i=1}^{n-1}a_k b_i = s_0\sum_{k=1}^{\infty}\sum_{n=k-1}^{\infty}\prod_{i=1}^{n-1}a_k b_i = s_0\sum_{k=1}^{\infty}\left\{\prod_{i=1}^{k-1}a_k b_i\underbrace{\sum_{n=k-1}^{\infty}\prod_{i=k-1}^{n-1}b_i}_{Eq.38}\right\} \quad (37)$$

The k^{th} term of the response function will be therefore multiplied by the following product of kernels:

$$\sum_{n=k-1}^{\infty}K_a(P_{n-1}\to P_n)\prod_{i=k-1}^{n-1}K_s(P_{i-1}\to P_i) \quad (38)$$

From *k* to *n* the chain of kernels are integrated without constraint for the detector domain, but now it can be calculated with relative ease. To show this, let us integrate the *n = k-1* and the *n = k*

terms, using the facts, that the kernels are normalized to 1 on the outgoing co-ordinate, and the absorption probability and the scattering probability add up to 1:

$$
\begin{aligned}
&(n=k-1): \int\int \int T\left(r_{k-2} \to r_{k-1} \mid E_{k-2}, \Omega_{k-2}\right) \frac{\Sigma_a\left(E_{k-2}, r_{k-1}\right)}{\Sigma_t\left(E_{k-2}, r_{k-1}\right)} dr_{k-1} dE_{k-2} d\Omega_{k-2} \\
&(n=k): \int \ldots \int\int T\left(r_{k-2} \to r_{k-1} \mid E_{k-2}, \Omega_{k-2}\right) \frac{\Sigma_s\left(E_{k-2} \to E_{k-1}, \Omega_{k-2} \to \Omega_{k-1} \mid r_{k-1}\right)}{\Sigma_t\left(E_{k-2}, r_{k-1}\right)} \times \\
&T\left(r_{k-1} \to r_k \mid E_{k-1}, \Omega_{k-1}\right) \frac{\Sigma_a\left(E_{k-1}, r_k\right)}{\Sigma_t\left(E_{k-1}, r_k\right)} d\Omega_{k-2} dE_{k-2} dr_{k-1} d\Omega_{k-1} dE_{k-1} dr_k =
\end{aligned}
\tag{39}
$$

$$
\begin{aligned}
&= \int\int T\left(r_{k-2} \to r_{k-1} \mid E_{k-2}, \Omega_{k-2}\right) \frac{\Sigma_s\left(E_{k-2} \mid r_{k-1}\right)}{\Sigma_t\left(E_{k-2}, r_{k-1}\right)} dr_{k-1} d\Omega_{k-2} dE_{k-2} - \\
&- \int\int T\left(r_{k-2} \to r_{k-1} \mid E_{k-2}, \Omega_{k-2}\right) \frac{\Sigma_s\left(E_{k-2} \to E_{k-1}, \Omega_{k-2} \to \Omega_{k-1} \mid r_{k-1}\right)}{\Sigma_t\left(E_{k-2}, r_{k-1}\right)} \times \\
&\times T\left(r_{k-1} \to r_k \mid E_{k-1}, \Omega_{k-1}\right) \frac{\Sigma_s\left(E_{k-1}, r_k\right)}{\Sigma_t\left(E_{k-1}, r_k\right)} d\Omega_{k-2} dE_{k-2} dr_{k-1} d\Omega_{k-1} dE_{k-1} dr_k
\end{aligned}
$$

The first term (*n = k-1*) of Eq.(39) added to the *(n = k)* –term will give 1 as a result, leaving behind a term when both the *k-1* -th and the k^{th} terms are scatterings. If the same procedure is made with the *n = k+1*-th integral, we will obtain the same form except the indices will be shifted. The remaining term will be cancelled out by a part the *n=k+1*-th term leaving behind the form, where the *k-1* -th the k^{th} and the *k+1*-th terms are all scatters. This can be applied recursively, and finally the infinite sum of these integrals yields 1.
The transport integral will look like - having changed the direction of the summation, and having repeated the same manipulation with the absorption term:

$$
\begin{aligned}
&\int \ldots \int \sum_{k=1}^{\infty} S\left(r_k\right) \Pi_{r \in V_d}\left(\underline{r}_0\right) \left\{ \Pi_{E_d, \Delta E_d}\left(\sum_{i=1}^{k-1} \Delta E_i^{\,s} \Pi_{r \in V_d}\left(\underline{r}_i\right) + \Delta E_0^{a} \right) - \Pi_{E_d, \Delta E_d}\left(\sum_{i=1}^{k-1} \Delta E_i^{\,s} \Pi_{r \in V_d}\left(\underline{r}_i\right) \right) \right\} \times \\
&K_a\left(P_1 \to P_0\right) \prod_{i=1}^{k-1} K_s\left(P_{i+1} \to P_i\right) dP_k \ldots dP_0 + \\
&+ \int \ldots \int \sum_{k=1}^{\infty} S\left(r_k\right) \Pi_{r \in V_d}\left(\underline{r}_0\right) \left\{ \Pi_{E_d, \Delta E_d}\left(\sum_{i=1}^{k-1} \Delta E_i^{\,s} \Pi_{r \in V_d}\left(\underline{r}_i\right) + \Delta E_0^{s} \right) - \Pi_{E_d, \Delta E_d}\left(\sum_{i=1}^{k-1} \Delta E_i^{\,s} \Pi_{r \in V_d}\left(\underline{r}_i\right) \right) \right\} \times \\
&\times \prod_{i=0}^{k-1} K_s\left(P_{i+1} \to P_i\right) dP_k \ldots dP_0
\end{aligned}
\tag{40}
$$

Now the sources of all terms are in the detector domain. For the complete adjoint simulation we have to cast Eq.(40) in the form described in Ref. 2 using the transition and collision kernels for the adjoint particle. If we look first to the integrand of the first term of Eq.(40) for a certain value of *k* we can write this term after integration over E_0 and W_0 as

$$S(P_k)\prod_{i=1}^{k-1} T(r_{i+1}\to r_i, E_{i+1}, \Omega_{i+1}) C_s(r_i, E_{i+1}\to E_i, \Omega_{i+1}\to \Omega_i) T(r_1 \to r_0, E_1, \Omega_1)\frac{\Sigma_a(r_0,E_1)}{\Sigma_t(r_0,E_1)}$$

$$= \frac{S(P_k)}{\Sigma_t(P_k)} T^+(r_{k-1}\to r_k, E_k, \Omega_k)\prod_{i=2}^{k-1} P^+(r_i, E_i) C^+(r_i, E_i \to E_{i+1}, \Omega_i \to \Omega_{i+1}) T^+(r_{i-1}\to r_i, E_i, \Omega_i) \quad (41)$$

$$\times P^+(r_1, E_1) C^+(r_1, E_1 \to E_2, \Omega_1 \to \Omega_2) T^+(r_0 \to r_1, E_1, \Omega_1)\Sigma_a(r_0, E_1)$$

with T^+ the adjoint displacement kernel, C^+ the adjoint scattering kernel and P^+ the adjoint weight factor [2]. To start the adjoint simulation we have to select $\boldsymbol{r}_0$ uniformly within the detector volume and W_1 isotropically. The energy E_1 should be sampled proportional to $S_a(\boldsymbol{r}_0,E_1)$, but it is more efficient to sample E_1 uniformly from the total energy range of interest and introduce a weight factor $S_a(\boldsymbol{r}_0,E_1)$. The functions $\Pi_{Ed,\Delta Ed}$ determine the deposited energy that is recorded during that history and thus determine the bin of the pulse height spectrum to which a score is made. A score is obtained when the adjoint particle has a collision in the original particle source (or crosses the source) with magnitude $S(P_k)/ S_t(P_k)$. Due to the Π term with a minus sign also a negative score must be recorded, but for a different deposited energy, as the arguments of the Π function differ.
The second term of Eq.(40) can be sampled almost the same way as the first term, except that the start of the simulation is different. The adjoint source term is determined by

$$T^+(r_0 \to r_1, E_1, \Omega_1) P^+(r_0, E_0) C^+(r_0, E_0 \to E_1, \Omega_0 \to \Omega_1)\Sigma_t(r_0, E_0) \quad (42)$$

This means that $\boldsymbol{r}_0$ is again selected uniformly within the detector volume, W_0 is selected isotropically, and E_0 is sampled uniformly from the total energy range of interest with a weight factor $S_t(\boldsymbol{r}_0,E_0)$. Then E_1 and W_1 are sampled from the adjoint collision kernel, and so on.

Another way of sampling Eq.(32) is to start again the adjoint simulation from the last collision in the detector, say at collision k. Then the next collisions will no more contribute to the deposited energy. As shown above the starting variables for the adjoint simulation are obtained by sampling $\boldsymbol{r}_0$ uniformly within the detector volume, W_0 isotropically, and E_0 uniformly from the total energy range of interest with a weight factor $S_t(\boldsymbol{r}_0,E_0)$. Moreover we have to include in the particle weight the probability that the forward particle leaves the detector after the collision at $\boldsymbol{r}_0$ into the direction W_0 and will not return to the detector. This probability can be estimated by a forward simulation starting at $\boldsymbol{r}_0$. This procedure has the advantage that there is no negative score. It is, however, not a pure adjoint simulation.

4. NUMERICAL EXAMPLE

To demonstrate the feasibility of such a game, a simplified form of the photon transport has been considered with only Compton-scattering and the photoelectric effect. The geometric model of the system consists of a 5-cm radius cylinder of 15-cm axis length. The photon source is a sphere of 2-cm radius emitting photons with a flat spectrum between 1.5 and 2 MeV. Its centre is located along the system axis, 5 cm from one outer end. The detector is a 0.25-cm radius sphere

with its centre 6 cm away from the other outer end of the system. The whole system has a uniform material composition. The Compton cross section is given by the Klein-Nishina formula with an amplitude of 0.1 cm^{-1}.The cross section for the photoelectric effect is taken inversely proportional to the third power of the photon energy with a value of 0.01 cm^{-1} at 1 MeV.

To check the results of the adjoint calculation a program was written to perform a forward calculation for this system. As the probability for a source photon to have an interaction in the detector is low, 10^9 photons were started at the source to obtain an accurate pulse height distribution of energy deposited in the detector.

The adjoint calculation was carried out based on the proposed methods in Ref. 2, also using 10^9 particle histories. The results of the forward and adjoint calculations can be seen in *Fig.1*. The pulse height distribution is registered in 50 energy bins of 0.04 MeV width up to 2 MeV.

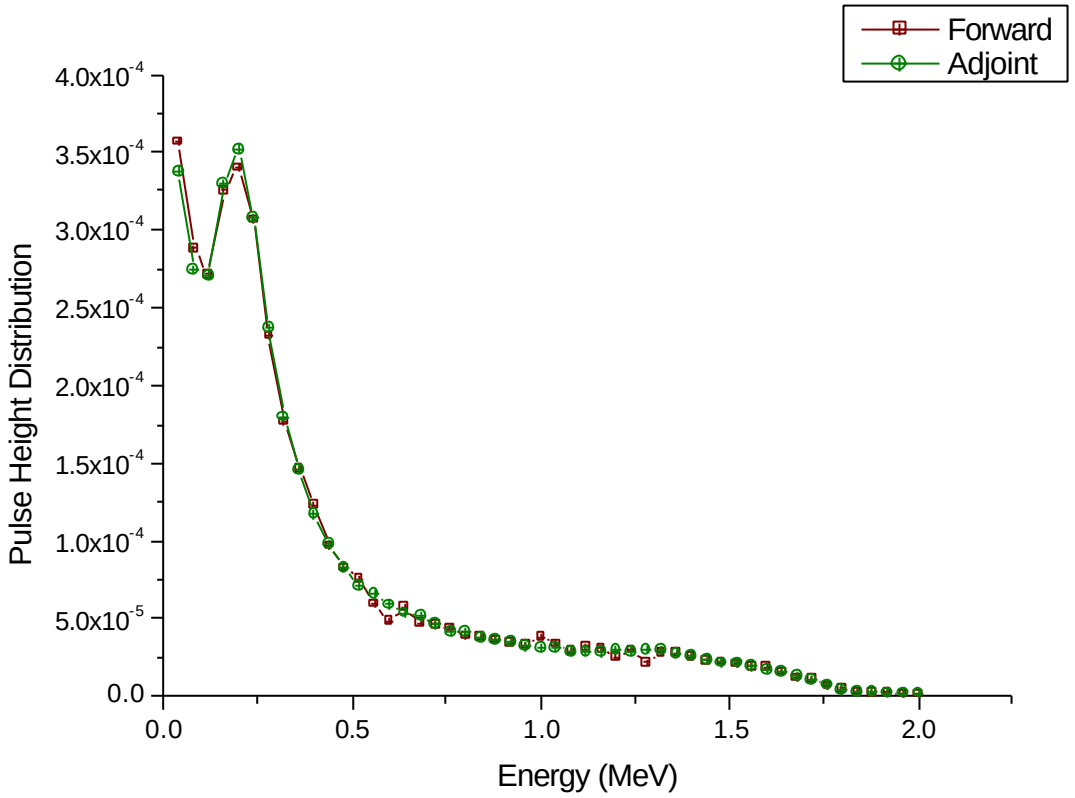

Figure 1. Pulse height distribution from adjoint and forward calculations

The results (*Fig. 1*) show good agreement between the adjoint and forward calculations, which demonstrates the validity of the theory presented here for adjoint estimation of a pulse height distribution.

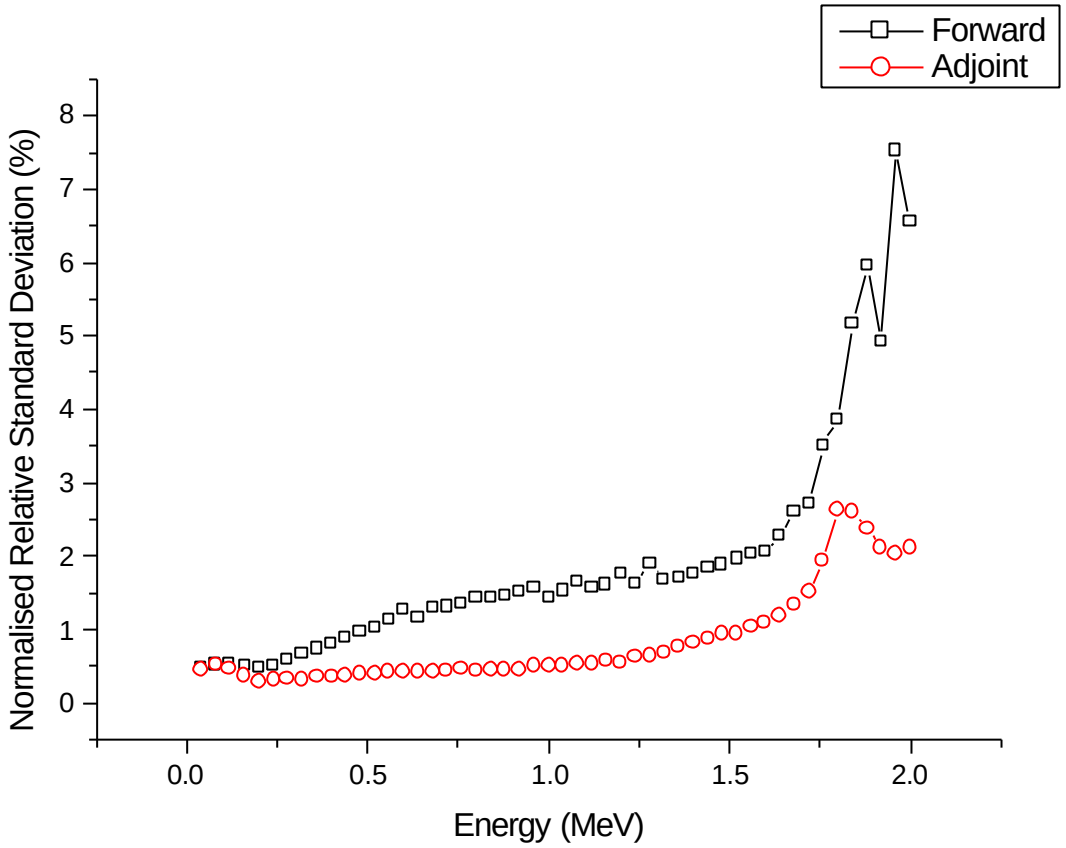

Figure 2. Comparison of effectiveness of the forward and the adjoint calculation

Figure 2 shows the relative standard deviation in each energy bin, both for the forward and the adjoint calculation. The standard deviations are normalised to a CPU time of 300 min both for the forward and the adjoint calculation. From *Fig. 2* it can bee seen that the adjoint calculation is more efficient than the forward calculation.

Figure 1. Pulse height distribution from adjoint and forward calculations

5. CONCLUSIONS AND DISCUSSION

It is shown that the distribution of total energy release of a particle can be estimated with adjoint Monte Carlo. A suitable formulation has been found that describes a non-multiplying Monte Carlo game and the possibility of a formulation for an adjoint game, with its source located in the detector only has been shown. The adjoint game was played with particles starting from the detector but the transformation of scoring –which allowed such sampling- led to positive and

negative contributions of particles to the response. For larger detectors where more than one collision is likely to happen in the detector, negative contributions will be made more frequently, resulting in higher variances, therefore this solution should be compared in the future to the method, when only positive scores are made, but the game is played partly with forward particles as indicated at the end of Sect. 3.

The sampling scheme is now valid only for systems without physical branching. An extension to processes with physical branching is suggested for further research. Also, possible forms for forward-adjoint coupling need to be established.

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