CHAIN SEGMENTATION FOR THE MONTE CARLO SOLUTION OF PARTICLE TRANSPORT PROBLEMS

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A Monte Carlo approach is proposed where the random walk chains generated in particle transport simulations are segmented. Forward and adjoint-mode estimators are then used in conjunction with the first-event source density on the segmented chains to obtain multiple estimates of the individual terms of the Neumann series solution at each collision point. The solution is then constructed by summation of the series.

The approach is compared to the exact analytical and to the Monte Carlo nonabsorption weighting method results for two representative slowing down and deep penetration problems. Application of the proposed approach leads to unbiased estimates for limited numbers of particle simulations and is useful in suppressing an effective bias problem observed in some cases of deep penetration particle transport problems.

INTRODUCTION

An approach to particle transport simulations by Monte Carlo is proposed. It depends on the formulation of forward and adjoint-mode estimators for the evaluation of the individual terms of the Neumann series solution to the Boltzmann transport equation. Each term is estimated separately, and the solution is then constructed by summing the series. The estimators are used in conjunction with a procedure of segmenting the random particle chains, which yields several estimates of the Neumann series terms at each collision point. In this paper, the results are compared to the exact analytical and the nonabsorption weighting Monte Carlo solutions for representative deep penetration and slowing down problems. Our objective is to gain a fundamental understanding of the proposed approach, leaving the comparison to other widely known Monte Carlo variance reduction methods for future research. Compared to the Monte Carlo method with nonabsorption statistical weighting, our approach offers an advantage: Estimation of the individual terms of the Neumann series, followed by their summation, highly suppresses an effective bias problem that is observed in some cases of deep penetration problems even though the theoretical bias is zero. This effective bias is thought to be due to undersampling of the probability space and improper normalization, when an insufficient number of particle histories are used. The generation of multiple estimates of the Neumann series terms at each collision point is a characteristic that may also be useful in complex geometry calculations where the generated chains involve a substantial investment in labor, and our approach extracts more information on these chains rather than generating new ones. The approach depends on the a priori analytical, numerical, or Monte Carlo determination of the first collision source for the treated problems.

The Monte Carlo method, using statistical weighting to account for absorption, is the most widely used method in current particle transport calculations and provides satisfactory results for many neutronics and photonics problems. However, such a method is inefficient in deep penetration problems for calculating radiation fluxes at large distances from the source, unless a large number of histories are used. For instance, in the work of Bending, one can notice that the solution is clearly underestimated at deep penetrations, and, moreover, the error bars fail to contain the true answer as shown in Fig. 1. This approach is improved by numerous variance reduction methods. However, even when biasing is used, as also shown in Fig. 1, some cases occur where the truth at deep penetrations is underestimated; even the error estimates are invalid, since they
clearly do not contain the truth. Our objective is to seek approaches for the elimination of this observed effective bias for limited numbers of particle histories. Stated differently, this work seeks approaches yielding unbiased and consistent estimators at deep penetrations. The further requirement of minimum variance in the estimators is left for future research.

The deep penetration problem is still a challenging area of active research. Gerstl has proposed new forms of the neutron transport equation for the solution of such deep penetration problems. Our work provides an interesting approach to this problem.

In the following sections, the theory of the proposed approach is outlined. Estimators for the individual terms of the Neumann series solution of the integral Boltzmann transport equation are derived. The proposed procedure of chain segmentation is explained. Our derived estimators are compared to other known estimators. The method is then applied to solve two-particle transport problems of interest, for which analytical solutions can easily be derived for the individual terms of the Neumann series. They are also compared to results of Monte Carlo with nonabsorption statistical weighting. Results of computations show that the undersampling problem leading to the previously mentioned effective bias occurring in deep penetration problems is highly suppressed by the present approach. For instance, in the case of Monte Carlo with no absorption weighting in one of our treated problems, and for media with \( \Sigma_d/\Sigma_t = 0.9 \), the result approaches the truth at deep penetrations (20 mfp) by increasing the number of generated chains from 100 to 1000, but still lies below it. Using our suggested approach, a better result is obtained with 100 histories than for the case of 1000 histories with an associated smaller expenditure in computing effort. The theory of the method and the numerical computations are exposed in the following sections. A brief background exposition is used to introduce the subsequent analysis.

**BACKGROUND**

Particle transport can be described by the integral form of the transport equation

\[
\phi(x) = S(x) + \int_R K(x \to y) \phi(y) \, dy,
\]

which can be a Fredholm or a Volterra equation of the second kind, depending on the problem at hand, where

\[
x = (r, E) = \text{six-dimensional vector in phase space} \\
R, \ \text{which can be split into the geometric space, the energy interval} \\
E(\text{min}) \to E(\text{max}), \ \text{and the velocity} \\
\Omega \ \text{direction space} \\
\]

\[
r = \text{spatial position vector} \\
E = \text{energy vector} \\
E = \text{particle energy} \\
\Omega = \text{unit direction vector} \\
y = (r', E') = \text{six-dimensional vector} \\
\phi(x) = \text{steady-state particle ingoing collision} \\
\text{density at } x \\
K(x \to y) = \text{kernel describing the particle transfer} \\
\text{probability from point } y \text{ to } x.
\]

The kernel \( K(x \to y) \) can be separated for convenience into fission, collision, and transport kernels so that

\[
K(x \to y) = K(r, E \to r', E') \\
= [C(E \to E'|r') + F(E \to E'|r')] \\
\times T(r \to r'|E). \tag{2}
\]
The fission kernel $F$ is the product of the fission yield factor $\nu(E)$, the energy distribution function of the emerging fission neutrons $\chi(E)$, and the fission cross section $\Sigma_f$ for the incident neutrons

$$F(E \rightarrow E'|r') = \nu(E')\Sigma_f(r',E')\chi(E) \quad (3)$$

The transport kernel $T$ expresses the spatial steps of particle transport:

$$T(r \rightarrow r'|E) = \Sigma_s(E) \exp[-\Sigma_t(E) \cdot d] \quad (4)$$

where $d$ is the distance from $r'$ to $r$.

The collision kernel $C$ describes elastic and inelastic scattering by the different laws of energy transfer and can be expressed as

$$C(E \rightarrow E'|r) = \sum_i p_i c_i(E \rightarrow E'|r) \quad (5)$$

with

$$p_i = \frac{\Sigma_{si}(E,E')}{\Sigma_t(E,E')}$$

and

$$c_i(E \rightarrow E'|r) = \frac{1}{4\pi} \Xi(E \rightarrow E'|r) \quad (6)$$

where

$\Sigma_s, \Sigma_t =$ scattering and total macroscopic cross sections, respectively

$\Xi =$ distribution of speeds following a collision for isotropic scattering.

The source term that describes the uncollided ingoing particle collision density to each space point from the external source is

$$S(r,E) = \int Q(r',E)T(r \rightarrow r'|E) dr' \quad (6)$$

where $Q(r',E)$ is the physical source density.

Since the composite kernel $K = (C + F)T$ will generally have a spectral radius very close to unity in the case of multiplying media, convergence of the corresponding Neumann series of the solution will be slow. To get a general method that can treat source nonmultiplying as well as source multiplying media and eigenvalue (criticality) problems, the kernel $K$ is split into two parts: $TC$ describes the nonmultiplying particle transport and the $TF$, all the neutron multiplying processes. Thus, Eq. (1) can be written as

$$\phi = S + (TC)\phi + (TF)\phi \quad (7)$$

It is obtained by splitting the last equation into a system of coupled integral equations of the form

$$\phi_i = S_i + (TC)\phi_i \quad (8)$$

which are all neutron transport equations for source problems for a nonmultiplying medium, where

$$S_i = TQ_i = S \quad (9)$$

and

$$S_i = (TF)\phi_{i-1}, \quad i = 2, 3, \ldots \quad (10)$$

The summation of all values of $\phi_i$ leads to

$$\sum_{i=1}^{N} \phi_i = (TC)\sum_{i=1}^{N} \phi_i + (TF)\sum_{i=1}^{N} \phi_i + S - (TF)\phi_N \quad (11)$$

If the system is subcritical, the sum

$$\sum_{i=1}^{N} \phi_i = \phi \quad (12)$$

becomes a solution for the collision density equation, and $(TF)\phi_N \rightarrow 0$ as $N \rightarrow \infty$. If, however, $\phi_{N-1}$ converges to $\phi_N$ as $N \rightarrow \infty$, then $\phi_N$ becomes a solution of the following homogeneous integral equation, which describes a just critical system,

$$\phi_N = (TC)\phi_N + (TF)\phi_N \quad (13)$$

The last procedure allows us to calculate characteristic multiplying media parameters. The ratio

$$k_i = \frac{\int_R S_i(x) dx}{\int_R S(x) dx} \quad (14)$$

is the multiplication factor between generations $(i + 1)$ and $i$. After some iterations, when the fundamental mode is reached, then $k_{i-1} = k_i$, $\phi_i = k_i\phi_{i-1}$, and

$$k_{\text{eff}}(\text{stat}) = \lim_{i \rightarrow \infty} k_i \quad (15)$$

becomes the parameter of stationary criticality. If $k_{\text{eff}} < 1$, the series for $\phi$ converges, and if $k_{\text{eff}} > 1$, the procedure diverges, since the system is supercritical, but the method can still be applied if an artificial reduction parameter is used.

The preceding discussion was intended to show that the solution of Eq. (1) that we attempt here can lead both to the solution of source and eigenvalue problems.

Equation (1) has an adjoint, which is

$$\phi^\dagger(x) = S^\dagger(x) + \int K^\dagger(x \leftarrow y)\phi^\dagger(y) dy \quad (16)$$

where

$$K(y \leftarrow x) \equiv K^\dagger(x \rightarrow y)$$
The following reciprocity relation links Eqs. (1) and (9):  

$$ \langle \phi, S \rangle = \langle \phi^t, S \rangle, $$  

where $\langle \cdot, \cdot \rangle$ denotes an inner product.

If $S^\dagger$ is chosen as a delta function, $\delta(y - x_{i_0})$, then we have  

$$ \phi(x_{i_0}) = \langle S, \phi^t \rangle = \langle \delta, \phi \rangle = \int \phi(y) \delta(y - x_{i_0}) dy. $$  

so that the solution at every point can be obtained from either a forward or an adjoint process. The theory of our proposed approach is exposed next.

**THEORY**

We choose a nonabsorbing Markov chain model as our underlying probabilistic model so that, for the forward-mode walk,  

$$ p(x, y) = \frac{K(x \leftarrow y)}{\int K(x \leftarrow y) dx}, $$  

implying a zero absorption probability,  

$$ p_s(y) = 1 - \int p(x, y) dx = 0, \quad \text{for all } y. $$

For the adjoint mode,  

$$ p^t(x, y) = \frac{K^t(x \leftarrow y)}{\int K^t(x \leftarrow y) dy}, $$  

implying a zero absorption probability,  

$$ p^t_s(x) = 1 - \int p^t(x, y) dy = 0, \quad \text{for all } x. $$

Equation (1) has an associated convergent Neumann series solution when  

$$ 0 < \int_R K(x \leftarrow y) dy < 1 $$

$$ E[\beta(\gamma_m)] = \int_{\gamma_m} \beta(\gamma_m) P(\gamma_m) d\gamma_m $$

$$ = \int_{x_m} \ldots \int_{x_1} \frac{K^t(x_{i_0}, x_{i_0}) K^t(x_{i_1}, x_{i_1}) \ldots K^t(x_{m-1}, x_{m-1})}{p(x_{i_0}, x_{i_1}) p(x_{i_1}, x_{i_2}) \ldots p(x_{m-1}, x_{m})} S(x_m) $$

$$ \times p(x_{i_0}) \ldots p(x_{m-1}, x_{m}) dx_{i_0} dx_{i_1} \ldots dx_m $$

$$ = \int_{x_m} \ldots \int_{x_1} K^t(x_{i_0}, x_{i_0}) K^t(x_{i_1}, x_{i_1}) \ldots K^t(x_{m-1}, x_{m-1}) S(x_m) dx_{i_0} dx_{i_1} \ldots dx_m $$

$$ = \langle S, K^m \delta \rangle $$

$$ = \int S(x) K^m(x, y) \delta(y - x_{i_0}) dx dy, $$
so that the value of
\[ \phi(x_{i_0}) = \langle S, \phi \rangle = \langle S, \delta + K^\dagger \delta + K^\dagger \delta + \ldots \rangle \]
can be obtained when the individual terms of the series are evaluated. Note that \( x_{i_0} \) is arbitrary in the general case. In the applications, we restricted ourselves to the cases where \( i_0 = i_0 \), although it is not a necessary choice. This means we are restricting ourselves to node points along the generated chains. In the general case, these points may lie out of the chains.

**Theorem II:** For the same conditions as Theorem I, and for a connected segment \( \gamma_m \) of length \( m \) of \( \gamma \), the random variable

\[ \theta(\gamma_m) = S(x_0) \frac{K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1}) K(x_{i_0}, x_m)}{p(x_1, x_0) p(x_2, x_1) \ldots p(x_m, x_{m-1})} \]

over a connected segment of length \( m \) is an unbiased estimator of the solution at \( x \) for the \((m + 2)\)th Neumann series term: \( \langle \delta, K^{m+1} S \rangle \), for all \( m > 0 \).

**Proof:** Taking the expectation of the random variable \( \theta(\gamma_m) \), conditional on \( x_0 \), we obtain

\[ E[\theta(\gamma_m)] = \int_{\gamma_m} \theta(\gamma_m) P(\gamma_m) \, d\gamma_m \]

\[ = \int_{x_m} \ldots \int_{x_0} S(x_0) \frac{K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1}) K(x_{i_0}, x_m)}{p(x_1, x_0) p(x_2, x_1) \ldots p(x_m, x_{m-1})} \]

\[ \times p(x_1, x_0) p(x_2, x_1) \ldots p(x_m, x_{m-1}) \, dx_0 \, dx_1 \ldots \, dx_m \]

\[ = \int_{x_m} \ldots \int_{x_0} S(x_0) K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1}) K(x_{i_0}, x_m) \, dx_0 \, dx_1 \ldots \, dx_m \]

\[ = \langle \delta, K^{m+1} S \rangle \]

\[ = \int \delta(x - x_{i_0}) K^{m+1}(x, y) S(y) \, dx \, dy . \]

**Theorem III:** Over an arbitrary forward nonabsorbing Markov chain \( \gamma \), and for an arbitrary connected segment \( \gamma_m \) of the chain of length \( m \), the random variable

\[ \lambda(\gamma_m) = S(x_0) \frac{K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1})}{p(x_1, x_0) p(x_2, x_1) \ldots p(x_m, x_{m-1})} \]

is an unbiased estimator of \( \langle \delta, K^{m+1} S \rangle \).

**Proof:** The proof proceeds as for Theorem II, except that our chain probability was longer by one step. In a sense Theorem II is a next-event-type estimator over the segments of the chains, whereas Theorems I and III are not.

Note that the whole approach depends on obtaining estimates for the individual terms of the Neumann series for the solution, and constructing the solution by summing up these terms. Currently used Monte Carlo estimators in particle transport are distinctly different in that they attempt to estimate the complete series in one step. They do not estimate each individual term of the series prior to its summation. The preceding theorems provided estimates for the Neumann series terms possessing the following properties:

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1. An arbitrary index \( i_0 \), which can be chosen over the chain or out of it. We confined ourselves to points on the chain, leaving the other alternative for future studies.

2. The chain probability can also be chosen without restriction, except the conditioning on its starting point, for example, as connected segments over a larger chain. This requires the first collision source \( S(x) \) to be determined by any method, including Monte Carlo, and the underlying Markov chain model to be a nonabsorbing one. This first collision source is sampled uniformly in this work.

3. The last three theorems pertain to forward-mode-generated random walk chains, over which we estimate either in an adjoint- or forward-mode manner.

The following theorems offer the analogous estimators to those of the preceding theorems with the estimation procedure superimposed over an adjoint-mode random walk. They are given without proofs, since the proofs are similar to those previously outlined.

**Theorem IV:** Over an adjoint arbitrary nonabsorbing Markov chain \( \gamma \), and for an arbitrary
connected segment \( \gamma_m \) of the chain of length \( m \), the random variable

\[
\beta^\dagger(\gamma_m) = \frac{K^\dagger(x_1, x_0) K^\dagger(x_2, x_1) \ldots K^\dagger(x_m, x_{m-1})}{p^\dagger(x_1, x_0)p^\dagger(x_2, x_1) \ldots p^\dagger(x_m, x_{m-1})} S(x_m)
\]

is an unbiased estimator for the solution at \( x_0 \) for the \( (m+1)^{st} \) term of the Neumann series: \( \langle S, K^{m+1} \rangle \) for all \( m > 0 \).

**Theorem V:** Over an adjoint arbitrary nonabsorbing Markov chain \( \gamma \), and for an arbitrary connected segment \( \gamma_m \) of length \( m \), the random variable

\[
\beta^\dagger(\gamma_m) = S(x_0) \frac{K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1})}{p(x_1, x_0)p^\dagger(x_2, x_1) \ldots p^\dagger(x_m, x_{m-1})}
\]

is an unbiased estimator of the solution at \( x \) for the \( (m+2)^{nd} \) term of the Neumann series: \( \langle S, K^{m+2} \rangle \) for all \( m > 0 \).

**Theorem VI:** Over an arbitrary adjoint nonabsorbing Markov chain \( \gamma \), and for an arbitrary connected segment \( \gamma_m \) of the chain, the random variable

\[
\lambda^\dagger(\gamma_m) = S(x_0) \frac{K(x_1, x_0) K(x_2, x_1) \ldots K(x_m, x_{m-1})}{p(x_1, x_0)p^\dagger(x_2, x_1) \ldots p^\dagger(x_m, x_{m-1})}
\]

is an unbiased estimator of the solution at \( x \) for the \( (m+1)^{st} \) term of the Neumann series: \( \langle S, K^{m+1} \rangle \) for all \( m > 0 \).

The preceding three theorems estimate separate individual terms of the Neumann series over connected segments of a larger underlying chain assuming the knowledge of the first collision source density \( S(x) \). The underlying chains there were generated in the adjoint mode, while the estimation over it can be either in the forward or adjoint mode.

In practical applications, a single chain can contribute several estimates to each individual term of the Neumann series at each collision point by the use of any of these estimators, as shown later. The choice of whether to generate a forward- or adjoint-mode basis chain may be problem dependent and is related to the source-detector configurations. Both forward- and adjoint-mode estimators can be used over these generated basis chains. For the same problem, forward- and adjoint-basis chains can be also generated, with chain segmentation and estimation over the segments either in the forward or adjoint modes.

**ESTIMATION PROCEDURE**

The following estimation procedure is suggested using the derived estimators.

1. According to either Eq. (12) or (13), a nonabsorbing random chain is generated. Consider a single chain of length \( M \):

\[
\gamma_M = (x_0, x_1, x_2, \ldots, x_M)
\]

with chain probability

\[
P(\gamma_M) = p(x_1, x_0)p(x_2, x_1) \ldots p(x_M, x_{M-1})
\]

2. For \( m = 0 \), take \( x_0 = S_{j_0}, i_0 = 1, 2, \ldots, M \). This is for the contributions of the source term.

3. For \( m = 1, 2, \ldots, M \), the chain is subdivided into connected segments of lengths \( m \).

   a. For an index \( x = j_0 \) sweeping the node points of the original chain, the segments of lengths \( m \) give multiple estimates of the \( (m+1)^{st} \) term of the Neumann series for each \( m \). There are different procedures for subdividing the chains. Figures 2a and 2b show one such procedure.

   b. By using any of the derived estimators, for example, that of Theorem I which estimates in an adjoint manner over a forward-generated chain, we obtain estimates of

\[
\langle S, K^{m+1} \rangle
\]

as

\[
\frac{K^\dagger(x_{r+1}, x_r) K^\dagger(x_{r+2}, x_{r+1}) \ldots K^\dagger(x_{r+m}, x_{r+m-1})}{p(x_{r+1}, x_r)p(x_{r+2}, x_{r+1}) \ldots p(x_{r+m}, x_{r+m-1})} S(x_{r+m})
\]

If desired, other estimates over the same chain can be obtained using the estimator of Theorem III, which estimates in a forward manner over the same forward-generated chain the quantity

\[
\langle S, K^{m+1} \rangle = \langle S, K^m \rangle
\]

as

\[
\frac{K(x_{r+1}, x_r) K(x_{r+2}, x_{r+1}) \ldots K(x_{r+m}, x_{r+m-1})}{p(x_{r+1}, x_r)p(x_{r+2}, x_{r+1}) \ldots p(x_{r+m}, x_{r+m-1})}
\]

4. Add to the estimates of \( S_{j_0} \) to obtain the Neumann series summation, and return to step 3a.

d. Repeat step 3 until satisfied.

4. Generate a new chain by going to step 1.

We now compare our estimation procedure to that currently used in Monte Carlo particle transport simulations. We particularly consider the collision estimator. It estimates the fluence over regions or specified volumes as parts of the treated systems. Defining a \( j \)'th particle weight for a forward walk at the \( (m+1)^{st} \) collision in region \( u \) as

\[
v_{W_{j_u}} = \frac{S(x_0) K(x_1, x_0) K(x_2, x_1) \ldots K(x_{m-1}, x_{m-1})}{p(x_0) p(x_1, x_0)p(x_2, x_1) \ldots p(x_{m-1}, x_{m-1})}
\]

or equivalently, as an estimate of the \( (m+1)^{st} \) term of the Neumann series solution, the collision density
Fig. 2a. Our estimator with a nonabsorbing Markov chain model. Estimation in an adjoint manner over a forward-generated chain. Multiple extra contributions of different Neumann series terms are obtained at chain nodes.

 fluence estimator will estimate the fluence over a region \( v \) as

\[
\phi_v = \sum_{i=1}^{n} \sum_{m=0}^{\infty} \frac{\phi_{W/m}}{nV_v \Sigma_{T_v}}.
\]

(15)

where

\( \phi_v = \) fluence in region \( v \) [interaction/(cm\(^2\)-source particle)]

\( \phi_{W/m} = \) weight of the \( j \)'th particle scattering in region \( v \)

\( n = \) total number of histories generated

\( V_v = \) volume of region \( v \)

\( \Sigma_{T_v} = \) total macroscopic cross section in region \( v \).

A major characteristic of Eq. (15) is that it assumes complete sampling of the phase space in the
sense that to obtain the Neumann series solution, the Neumann series terms must occur with uniform frequency in different volumes of interest during the simulation. This means that Eq. (15) is assumed of the form

\[ \phi_0 = \frac{1}{n V_0 \Sigma V_0} \left( \frac{u_{n_0}}{n} \sum_{i=1}^{n} u_i W_i + \frac{u_{n_1}}{n} \sum_{i=1}^{n} u_i W_i + \ldots \right) , \]

where

\[ \frac{u_{n_i}}{n} = 1 . \]

In the limit of complete sampling of the sample space, or when \( n \to \infty \), one can expect \( u_{n_0} = u_{n_1} = u_{n_2} = \ldots = n \), and we get the right estimate for the Neumann series solution. Unfortunately, this is not the case occurring in practice unless an unreasonably and impractically large number of histories are used. What usually happens is that

\[ u_{n_0} = u_{n_1} = u_{n_2} = \ldots = \alpha \]

and in some cases, some of the values of \( u_{n_i} \) are simply zero. At deep penetrations, those values of \( u_{n_i} \) with large values of \( i \) usually are smaller than the values of \( n_i \) with small values of \( i \), and an underestimation of the particle fluence can be expected (and actually happens in practice). These remarks have been supported by our numerical calculations, and the anticipated effects were reported in previous work as "undersampling" and "effective bias" by other authors.\(^{11}\) We are also indebted to one of the reviewers for the observation that this analysis may also explain the fact that "undersampling may lead in some cases to gross overestimates." This may occur in situations where the high-order terms of the Neumann series are not adequately sampled, and the lower order terms are the ones mostly contributing to the answer for limited numbers of histories. In our numerical cases, however, we met the reverse situation where the low-order terms were undersampled at deep penetrations.

To avoid the above-mentioned undersampling and normalization problems, the characteristic of our approach, which depends on obtaining multiple estimates of the Neumann series terms at each collision point of a chain, is used to estimate each term separately and then summing up the series. We can thus obtain not only the right normalization, but also several estimates of Neumann series terms at each node point of the chain, rather than a single estimate of one single term only at each node point. Thus, the following secondary estimator over each region is used:

\[ \phi_0 = \frac{1}{V_0 \Sigma V_0} \sum_{i=0}^{m} I_i , \quad I_i = \sum_{j=1}^{\frac{m}{u_{n_i}}} \frac{I_{i_j}^u}{u_{n_i}} , \]

where

\[ m = \text{maximum considered chain length} \]

\[ I_{i_j}^u = \text{estimate of the } i^{th} \text{ Neumann series term in region } u \text{ from the primary estimators exposed in our theorems} \]

\[ u_{n_i} = \text{number of estimates of the } i^{th} \text{ Neumann series term in region } u \text{ obtained by our primary estimators from the theorems} \]

\[ I_{i_j} = \text{i}^{th} \text{ estimate of the } i^{th} \text{ Neumann series term in region } u . \]

Thus, our approach estimates and sums separately each individual term of the Neumann series, calculates an average value for each term, and then sums them up to construct the solution. If some terms do not occur in a given simulation, interpolation between the other terms can give an estimate for them. This is, in fact, a generalization of the commonly used Eq. (15). Only when the number of particle histories tends to infinity, implying a complete sampling of phase space, can one expect on the average each term of the Neumann series to occur:

\[ \frac{1}{I \cdot n} \]

times in each region, where \( n \) is the number of histories and \( I \) is the average maximum chain length. Consequently, our estimator of Eq. (16) will tend to that of Eq. (15). However, since, in practical applications, the number of generated chains can never be large enough for the individual Neumann series terms to occur uniformly over each defined geometry region, application of our estimator Eq. (15), even in applications of Monte Carlo, not including our presently analyzed approach, will obviously avoid a significant bias in the answer.\(^{11}\) Our numerical results show that even though more labor per generated chain is involved in our approach, a much better result can be obtained with smaller computer time requirements than the Monte Carlo method with nonabsorption weighting, provided the first collision source is known. The latter can be estimated itself by Monte Carlo with a large number of histories to assure sufficient accuracy. The same order of accuracy needed by our method is also needed by other methods, in the estimate of the first collision source, for accurate results. So its estimation in our method does not really jeopardize the estimation process. As a matter of fact, an advantage of our method is to oblige us to obtain an estimate of the first collision source with sufficient accuracy, which is always needed regardless of the method being used. In the Monte Carlo with nonabsorption weighting case, this requires a sufficiently large number of histories. It can also be estimated analytically, by collision probability, weighted residual, or finite difference methods.
Methods of determining the first collision source by Monte Carlo are discussed in Ref. 17. A comparison of the proposed approach with previous related work is exposed in the Appendix.

**MODEL PARTICLE TRANSPORT PROBLEM I**

Problem Formulation: Slowing Down in Hydrogen or Particle Transmission Through a Slab Shield with Asymmetric Collisions

We consider the problem of neutrons slowing down in hydrogen with scattering and absorption cross sections $\Sigma_s$ and $\Sigma_a$ assumed constant, the source being at zero lethargy and monoenergetic. The object of the calculation is the determination of the slowing down density $\psi(x)$ as a function of $x$. The resonance escape probability is the slowing down density per unit source, at the thermal lethargy $x = T$. The problem is physically equivalent to that of a monoenergetic beam of particles (neutrons or gamma rays), normally incident on an infinite slab shield with constant cross sections $\Sigma_s$, $\Sigma_a$, and $\Sigma_t$, but the result of each collision event being absorption or undeflected straight-ahead progress into the shield. The objective of the calculation is the determination of the spatial attenuation of the impinging beam $\psi(x)$. The shield transmission probability through a thickness of $x = T$ mean-free-paths will be $\psi(T)$. Both of these problems are represented by the following integral equation for $\psi(x)$, which is a Volterra equation of the second kind:

$$\psi(x) = S(x) + \int_0^x K(x,y)\psi(y) \, dy, \quad 0 \leq x \leq \infty ,$$

(17)

where $x$ extends over the positive real line. The kernel is interpreted as: if $y$ then $x$ with probability density $K(x,y)$.

Let us consider the problem described mathematically as

$$S(x) = e^{-x}, \quad 0 < x < \infty$$

(18)

$$K(x,y) = \begin{cases} \frac{\Sigma_s(x)}{\Sigma_t(x)} \exp[-(x-y)], & 0 < y < x < \infty, \\ 0, & 0 < x < y < \infty \end{cases}$$

(19)

Note that

$$K_t(x,y) = K(y,x) = \frac{\Sigma_s(y)}{\Sigma_t(y)} \exp[-(y-x)] ,$$

where $S(x) = \text{first-event source}$

$K(x,y) = \text{kernel that does not allow backward steps}$

In the present case, $K(x,y)$ is factorable as

$$K(x,y) = C(x) \cdot T(x,y) ,$$

where

$$C(x) = \frac{\Sigma_s(x)}{\Sigma_t(x)} = \text{collision kernel}$$

$$T(x,y) = \exp(-x-y) = \text{transport kernel} .$$

The same problem has previously been considered as a model problem in different contexts by MacMillan and by Covley and others. They also analyzed a special case of it that can be regarded as considering the infinite positive real line as divided into two regions: the first of thickness $T$ partly scattering and absorbing (i.e., $\Sigma_a/\Sigma_t, \Sigma_s/\Sigma_t \neq 0$), and the second as extending from $T$ to infinity totally absorbing ($\Sigma_a/\Sigma_t = 0$). Our treatment considers a single region extending over the real positive line, partly scattering and absorbing such that $\Sigma_a/\Sigma_t + \Sigma_s/\Sigma_t = 1$.

**Analytical Solution for the Neumann Series Terms**

We seek to deduce the analytical solution for the Neumann series terms of the problem formulated by Eqs. (17) through (20) for future comparison to our proposed approach and to Monte Carlo with nonabsorption weighting. Equation (17) has the Neumann series solution:

$$\psi(x) = S(x) + \sum_{n=1}^{\infty} J_n(x) ,$$

where

$$J_n(x) = \int \cdots \int L_n(x,y_1,y_2,\ldots,y_n) \, dy_1 \, dy_2 \cdots dy_n$$

$$L_n(x,y_1,y_2,y_3,\ldots,y_n) = K(x,y_n)K(y_n,y_{n-1})\cdots K(y_2,y_1)S(y_1) ,$$

$n = 1,2,3,\ldots$.

Here, we use the forward estimator of Theorem III. Substituting for $S(x)$ and $K(x,y)$ from Eqs. (18) and (19) into Eq. (17), we find

$$\psi(x) = e^{-x} + \int_0^x \psi(y) \frac{\Sigma_s(y)}{\Sigma_t(y)} \exp[-(x-y)] \, dy ,$$

$$0 < x < \infty .$$

(21)
Thus,
\[ L_n(x) = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^n \exp\left(-x - y_n \right) \exp\left(-y_1 - y_{n-1} \right) \]
\[ \ldots \exp\left(-y_2 - y_1 \right) \exp\left(-y_1 \right) = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^n e^{-x}. \]

We can estimate the Neumann series terms. For \(0 < x < \infty\),
\[ I_0 = e^{-x} \]
\[ I_1 = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{1} e^{-x} \int_0^x dy_1 \]
\[ I_2 = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{2} e^{-x} \int_0^x \int_0^{y_1} dy_1 dy_2 \]
\[ \ldots I_n = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{n} e^{-x} \int_0^x \int_0^{y_1} \ldots \int_0^{y_{n-1}} dy_1 dy_2 dy_3 \ldots dy_n \]

By direct integration, we get
\[ I_0 = e^{-x} \]
\[ I_1 = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{1} e^{-x} \frac{x}{1} \]
\[ I_2 = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{2} e^{-x} \frac{x^2}{2!} \]
\[ \ldots \]
\[ I_n = \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{n} e^{-x} \frac{x^n}{n!} \]

The following recurrence relation is satisfied:
\[ I_{n+1} = I_n \left( \frac{\Sigma_i}{\Sigma_{i'}} \frac{x}{n+1} \right) \]

Summing up the series, we obtain
\[ \psi(x) = \sum_{i=0}^{\infty} I_i \]
\[ = e^{-x} \left[ 1 + \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{1} \frac{x}{1!} + \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{2} \frac{x^2}{2!} + \ldots + \left( \frac{\Sigma_i}{\Sigma_{i'}} \right)^{n} \frac{x^n}{n!} + \ldots \right] \]
\[ = e^{-x} \exp(\Sigma_i \Sigma_{i'}) \cdot x \]
\[ = \exp(-1 - \Sigma_i \Sigma_{i'}) \cdot x \]
\[ \psi(x) = \exp\left(-\Sigma_i \Sigma_{i'} \cdot x \right), \quad 0 < x < \infty. \]

Note here that \(x\) is measured in units of mean-free-paths.

Monte Carlo Solution

As the probability density function for our generated chains we choose
\[ p(x, y) = \frac{T(x, y)}{\int_y^\infty T(x, y) \, dx} = \frac{\exp[-(x - y)]}{\int_y^\infty \exp[-(x - y)] \, dx} \]
\[ = \frac{\exp[-(x - y)]}{\exp[-(x - y)]} = \exp(-\Delta l), \]

where \(\Delta l = x - y\), and the transport kernel is normalized.

Since the transport kernel is normalized, this implies a nonabsorbing Markov chain model. The cumulative distribution function for \(p(x, y)\) is
\[ D(x, y') = \int_{y'}^x \frac{T(x', y) \, dx'}{\int_y^\infty T(x', y) \, dx'} = \frac{\exp[-(x' - y)] \, dx'}{\exp[-(x' - y)] \, dx'} \]
\[ = 1 - \exp[-(x' - y)] = 1 - \exp(-\Delta l) = \rho, \]

so that generating uniform random numbers over the unit interval enables us to sample positions \(x_i\) of the colliding particle over the interval \([0, \infty)\) as
\[ x_i = x_{i-1} + \Delta l_i, \]

where
\[ \Delta l_i = -\ln(1 - \rho_i) = -\ln\rho_i. \]

Here, we replace \((1 - \rho_i)\) by \(\rho_i\), since they are both uniformly distributed over the unit interval.

We choose to consider the variable \(\Delta l\), since it is the incremental distance to the next collision that is customarily sampled in particle transport simulations. The chains were truncated when the statistical weight of the particle fell below a certain small preset value, or after a certain predetermined number of collisions, whichever happened first. This approach was favored to the use of Russian roulette for the termination of particle histories. The objective was to test the approach with respect to the elimination of the effective bias and to compare the numerical and analytical values of the individual Neumann series terms, without consideration of the further effect introduced by the importance sampling nature of the Russian roulette procedure. The chains were segmented so that for a chain of length \(M\), we obtained \((M - m + 1)\) estimates for each \(m\)th term of the Neumann series. Penetrations of 40 mfp were considered in our numerical computations.

Comparison of Results

As a first step, we solved the above-mentioned problem using the commonly used collision estimator
with nonabsorption weighting. A maximum chain length of 30 was used, and we compared the result to the analytical result. Figures 3 and 4 show this comparison for the case

\[
\frac{\Sigma_e}{\Sigma_t} = 0.9
\]

for different numbers of histories. The Monte Carlo result is shown in histogram form averaged over ten regions, while the analytical result is shown as a solid line. Figure 3 shows that for high absorption

\[
\left( \frac{\Sigma_e}{\Sigma_t} = 0.9 \right)
\]

the ordinary collision estimator, clearly underestimates the answer. The underestimate corrects itself when the number of histories is increased, as shown in Fig. 4, but is still below the truth for a rather large number of histories. Applying our approach, as shown in Figs. 5 and 6, drastically corrects the answer, and, moreover, does so with less time consumption. Our 100 histories result [9.6 s of central processor unit (CPU) time] and also our 10 histories (8.2 s), clearly give superior results to the common collision estimator for 10,000 histories (1 min, 4 s). Table I further shows the result obtained with our method by a case with 1000 histories and compares it to the collision estimator and to the exact analytical results. The ordinary collision estimator completely fails to obtain the right order of magnitude for the solution at deep penetrations for moderate numbers of histories, while our proposed approach achieves it successfully.

The CPU time reported includes the use of routines for displaying the results on graphics terminals and for plotting the results and must be considered in a relative sense.

Table II shows the distribution of the number of contributions to the individual Neumann series terms in each region. We have 31 Neumann series terms, since our chosen chain length was 30. In region 1, few estimates of the higher order terms are obtained, while in the tenth region, the lower order terms contributed \( \sim 25 \) estimates to each Neumann series.
Fig. 5. Comparison of exact and new forward estimator solutions, \( N = 10 \) histories.

Fig. 6. Comparison of exact and new forward estimator solutions, \( N = 100 \) histories.

**TABLE 1**

Comparison of Collision and New Estimators, \( \Sigma_e/\Sigma_t = 0.9 \)

<table>
<thead>
<tr>
<th>Region</th>
<th>( x ) (mfp)</th>
<th>Analytic*</th>
<th>Collision Estimator</th>
<th>New Estimator</th>
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*Analytic results are average values integrated over each region.
*Read as \( 2.7019 \times 10^{-1} \).
TABLE II
Distribution of Contributions to Neumann Series Terms over Different Regions—New Forward Estimator
(Chain length = 30 and number of chains = 100)

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Model Particle Transport Problem II

Problem Formulation: The One-Speed Transport Equation for a Plane Source at the Origin in an Infinite Homogeneous Medium

We sought another particle transport problem with an analytical solution for the purpose of comparison to our approach, and to the commonly used Monte Carlo method with nonabsorption weighting. Numerical methods were avoided at the present time, since they are known to contain their own sources of errors, and the objective of our work is to try to
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*Read as 0.2398 \times 10^{00}.

Eliminate or suppress the magnitude of biases appearing in transport problems. However, very few problems possess an exact analytical solution. Some of the most difficult ones possessing an analytical solution were treated by Case et al., and include point and plane sources in infinite media with isotropic and anisotropic scattering. We choose the one-speed transport problem of a plane source at the origin in an infinite homogeneous medium with isotropic scattering in the laboratory system. The same problem was used by Drawbaugh for comparison to the results of conditional Monte Carlo for the solution of particle transport problems. Here we use the tabulated results given by Drawbaugh for purposes of comparison. Generalization to multi-speed problems and to finite heterogeneous media will be the subject of future work and will have to include comparison to finite difference methods solutions, or to experiments.

The one-speed transport equation for a plane source at the origin in an infinite homogeneous medium with isotropic scattering in the laboratory system is for the flux:

$$\phi(x) = \frac{1}{2} E_1(|x|) + \frac{C}{2} \int_{-\infty}^{+\infty} E_1(|x - y|) \phi(y) \, dy,$$

with $E_1(x)$ as the exponential integral.
III

Different Regions—New Forward Estimator

chains = 100, and $\Sigma_0/\Sigma_t = 0.9$

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\[ E_i(x) = \frac{\exp(-xt)}{x} \int_{x_1}^{\infty} \frac{dx}{t} \quad (23) \]

and where $c = \Sigma_0/\Sigma_t$ is the ratio of macroscopic scattering to total collision cross section.

The Neumann series solution to the problem is

\[ \phi(x) = \frac{1}{2} E_1(|x|) + \sum_{i=1}^{\infty} I_i(x) \]

\[ I_i(x) = \left( \frac{3}{2} \right)^{i-1} \int_{x_1}^{\infty} \ldots \int_{x_{i-1}}^{\infty} E_1(|x-x_1|) E_1(|x-x_2|) \ldots E_1(|x-x_i|) \, dx_1 \, dx_2 \ldots dx_i \]

Since $I_i(x) = I_i(-x)$, only $I_i(|x|)$ is considered. In this problem, we only considered the truncated Neumann series

\[ I_0(x) + \sum_{i=1}^{20} I_i(x) \]

since Drawbaugh only gives analytical results for that range.

\[ \text{Monte Carlo Solution and Comparison of Results} \]

As a first step, the behavior of the solution by analog Monte Carlo with nonabsorption weighting
was studied, since this is the most widely used method in Monte Carlo calculations. The first 20 mfp from the source was divided into 20 regions and the scores accumulated over each, using the collision estimator. Figure 7 shows the behavior of the solution for a highly absorbing medium

$$c = \frac{\Sigma f}{\Sigma r} = 0.1$$

for a number of histories (5, 100, 5000, and 100000). Table IV shows the computational statistics. As already discussed, the result is always underestimating the truth for moderate numbers of histories. The Monte Carlo result approaches the truth when the number of histories used is increased. For a highly absorbing medium ($c = 0.1$) as shown in Fig. 7d, even with 100000 histories, at a relative cost of $17$, the answer from 8 to 20 mfp is still underestimating the truth. This shows that as conventionally used, the Monte Carlo method with nonabsorption weighting can eventually lead to the truth, but unfortunately, at the expense of a large number of histories. When a small number of histories are used as imposed by computer cost limitations, a situation arises in which the undersampling and the normalization of the Neumann series terms may lead to underestimation of the truth. The situation is made doubly dangerous for an unsuspecting user if he does not check the convergence of his results, in that the error bars will also give a wrong estimate of the error with a false confidence in the results for the user. Rather than using a Russian roulette procedure, we followed the particles to a lower weight of $1.0 \times 10^{-20}$, which amounts to truncation of the Neumann series.

Our method was then applied, where we generated chains and segmented them to apply our deduced estimators $\beta$ and $\lambda$ of Theorems I and III. The individual terms of the Neumann series were then evaluated in each region, and their sum added up to construct the solution. The maximum chain length
was determined by the particle's weight falling below $1.0 \times 10^{-26}$, or the chain length being 30, whichever happened first. The first collision source term for this particular problem is known. Its determination by Monte Carlo is studied in Ref. 17.

Figure 8 shows results of application of our suggested approach using our adjoint-mode estimator $\beta$ of Theorem I for a highly absorbing medium. Figure 9 shows the results for the forward-mode estimator $\lambda$ of Theorem III, while Fig. 10 shows the results of both estimators being used to estimate individual terms of the Neumann series. Table IV shows the computation statistics for the treated cases of 5, 10, 100, 1000, and 5000 histories. For $c = 0.1$, as shown in Figs. 8b and 9b, the exact solution is attained when using only ten histories at a relative cost of $0.56$. This is a very marked improvement over the Monte Carlo method with nonabsorption weighting, where a much inferior result was obtained, as shown in Fig. 7d with the use of histories at the expense of a relative cost of $17.1$. Comparing Figs. 8, 9, and 10 shows that no major improvement has been obtained by using both the forward- and adjoint-mode estimators. Using one is quite sufficient for the treated problem. This implies that after a certain limit, obtaining further extra estimates of the Neumann series terms is no more beneficial, and a recourse to a sequential sampling technique to stop the sampling, when no more are needed, is advised. This also applies to the total number of generated chains, since ten histories were quite enough to obtain an adequate result, and increasing the number of histories to 5000 in one of our treated cases was unnecessary. Further computational results are reported in Ref. 1.

CONCLUSIONS AND RECOMMENDATIONS

A Monte Carlo approach is proposed for the solution of Volterra and Fredholm equations of the
### TABLE IV
Computational Statistics for Different Methods

$(\Sigma_i / \Sigma_v = 0.1$, lower attainable weight for particles $= 1.0 \times 10^{-26}$, and maximum number of Neumann series terms $= 30$)

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<td>0.20</td>
<td>0.58</td>
<td>0.25</td>
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<td>0.58</td>
<td>0.82</td>
<td>0.37</td>
<td>1.60</td>
</tr>
<tr>
<td>1000</td>
<td>2 min, 10.5 s</td>
<td>3.43</td>
<td>2.33</td>
<td>1.05</td>
<td>4.83</td>
</tr>
<tr>
<td>5000</td>
<td>10 min, 12.1 s</td>
<td>16.07</td>
<td>9.02</td>
<td>4.08</td>
<td>20.15</td>
</tr>
</tbody>
</table>

Second kind, with special emphasis on application to particle transport in slowing down and deep penetration shielding problems.

The approach depends on derived forward and adjoint estimators with an underlying forward or adjoint nonabsorbing Markov chain model. It addresses itself to estimating individual terms of the Neumann series of the solution and constructs the final solution by adding up the individual components, by an approach different than currently used in Monte Carlo general purpose codes. The method uses a procedure of chain segmentation to obtain many more estimates of the Neumann series terms at each collision point than is obtainable by the commonly used collision estimator, and obtains at the expense of extra labor and the prior determination of the first collision source more information on a given chain than by using the common collision estimator.

Model problems for particle slowing down, or transmission through a shield have shown the promising capabilities of the method, by comparison to the Monte Carlo method with nonabsorption weighting. Deep penetration problems where further estimates for the lower order terms of the Neumann series are needed at deep penetrations, and complex geometries, problems where extraction of possible information at collision points may be more advantageous than generating new chains, are potential areas for the beneficial application of the exposed approach.

We are indebted to the reviewers for useful comments on the further extension of the present investigation. Future research should include interesting comparisons with calculations involving biasing.
Fig. 8a. Comparison of new method with forward estimator to exact solution, $N = 5$.

Fig. 9a. Comparison of new method with adjoint estimator to exact solution, $N = 5$.

Fig. 8b. Comparison of new method with forward estimator to exact solution, $N = 1000$.

Fig. 9b. Comparison of new method with adjoint estimator to exact solution, $N = 1000$. 

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and importance sampling methods, and including various standard estimation schemes. This will lead to the deduction of estimators that are not just unbiased and consistent, but are also of a minimum variance nature. This last requirement has not been addressed in the present work. Estimators for the variance of the proposed estimators need to be developed. There is a need for the identification of the mechanisms for the apparent improvements achieved by the proposed approach: How much improvement can be assigned to the chain segmentation and attainment of multiple estimates of the Neumann series terms, to the estimation of the first event source, and to the normalization inherent in the used secondary estimators, respectively? The approach also needs to be tested for more realistic problems for which analytical solutions do not exist, for instance, the determination of the total current through a thick iron slab due to a normally incident monoenergetic source, with comparison to numerical or experimental results. In this type of problem, higher order collisions dominate the contribution to the total current. Further studies would help establish the merits of the proposed approach and determine whether the implementation of such new approaches is a satisfactory solution to many difficult shielding problems, or whether "the real satisfactory solution to these problems is just faster computers designs."

APPENDIX

COMPARISON WITH PREVIOUS WORK

General Considerations

The proposed method uses a nonabsorbing Markov chain probability model and subdivides the generated chains into connected segments. By a knowledge of the first collision source, obtained by Monte Carlo or other methods, the method tries to gather several contributions to the individual terms of the Neumann series of the solution at each collision point, whereas the widely used collision estimator method gathers only one single contribution at each collision point. By its nature, our method estimates individual terms of the Neumann series over each spatial region and constructs the solution by summing them. The currently used methods do not address themselves to estimating individual components of the Neumann series, except for the conditional Monte Carlo method as introduced by Drawbaugh. Currently used methods, when used for multiregion problems, unless an unreasonably large number of particle histories are processed, overestimate the solution at moderate penetrations and underestimate it at deep penetrations. It seems that this is due to an undersampling problem at deep penetrations and to an inadequate normalization.
procedure, which, for moderate numbers of processed particles, does not assign the right weighting to individual terms of the Neumann series solution. The undersampling problem is alleviated by our method, which obtains several contributions to many Neumann series terms at each collision point. By estimating the individual terms of the Neumann series, the right normalization is obtained even if a moderate number of particle histories are used. An extra bonus is obtained by informing us about the convergence of the Neumann series and by the possibility to interpolate for the terms which did not occur in certain areas of phase space in a given simulation.

These advantages are not free. For practical applications, extra labor is spent for the generation of the first collision density, for chain segmentation, and for scoring contributions to the individual terms of the Neumann series. The extra data manipulations require more memory storage than ordinarily used Monte Carlo methods, but still remain minor compared to finite difference methods, so that applications to complex geometry three-dimensional problems are still possible. In addition, for applications where the tracking of particles through a complex geometry is the bulk of the computational effort, application of our method is very promising. Another application of our method is deep penetration problems. Our model problems are of this category and show the capabilities of our method for such problems. Application of biasing methods for such problems is problematic, since it requires prior information about the solution to the problems it is solving. If the right biasing is not used, erroneous results are obtained without any warning to the user.26

Comparison to Next-Event Estimators

A literature survey reveals that one of our forward-mode primary estimators bears a resemblance to, but is different from the Kalos next-event and once more collided estimators. Kalos is interested in estimating particle fluxes at one or several points in particle transport, but he is not concerned about segmenting the chain and getting contributions to the different terms of the Neumann series at each collision point and does not need a knowledge of the first collision source. Since no history can be expected to carry a neutron through a point, Kalos uses analytical expected value estimates and depends on the relation between \( \psi(r,E,\Omega)dr'd\Omega \), the density of particles entering collisions in volume \( dr' \) with energy in \( dE \) and direction \( d\Omega \), and the flux at \( r \):

\[
\phi(r) = \int dE' \int dr' \int d\Omega \psi(r',E,\Omega) \\
\times 2g \left( \frac{r-r'}{|r-r'|} \cdot \Omega, E \right) \cdot \exp(-\mu(E')|r-r'|) \\
\times \frac{1}{4\pi |r-r'|^2}.
\]  

(A.1)

Fig. A.1. Kalos next-event estimation at a point \( P_0 \). Chain may go beyond point 4. Markov chain model may be nonabsorbing or absorbing.

where

\[
g(\omega;E)\,d\omega = \text{probability of scattering a neutron of energy } E \text{ through an angle whose cosine is in the range } (\omega, \omega + d\omega) \\
E' = \text{energy after scattering} \]

\[
\mu(E') = \text{total attenuation coefficient of the scattered neutron.}
\]

A comparison of Fig. A.1 to Fig. 2 demonstrates the different natures of these estimators. Interestingly, it can be observed that the present approach can be generalized to use next-event estimation for points lying outside the generated chain.

Comparison to the Albert Adjoint Estimator

The same literature survey also reveals a resemblance to our adjoint-mode estimators to an estimator introduced by Albert, and analyzed by Spanier and Gelbard, in the context of adjoint calculations and the estimation of particle fluxes at one or several points.

The random variable

\[
I_0 = S(P_0) + I^* 
\]

is an unbiased estimator of \( \psi(P_0) \), the collision density at point \( P_0 \), where

\[
I^* = \frac{S(P_n)K(P_{n-1},P_n) \ldots K(P_1,P_2)K(P_0,P_1)}{K^\dagger(P_n,P_{n-1}) \ldots K^\dagger(P_2,P_1)S^\dagger(P_1)P^\dagger(P_n)} \\
\times \prod_{i=1}^{n-1} c^\dagger(P_i) \\
S, K = \text{forward source and kernel \( \{K(P_0,P_1) = \)} \\
\text{if } P_1 \text{ then } P_0)]
\]

(A.2)
$S^\dagger, K^\dagger$ = adjoint source and kernel

$p_0, \ldots, p_n = $ collision points of the random walk that terminates at $p_n$

$c^\dagger(p)$ = multiplicative weight acquired upon collision at $p$, which can account for multiplication by the presence of $c^\dagger(p)$, and where the walk is terminated at $p$, with probability $p^\dagger(p)$ or is continued with probability $q^\dagger(p) = 1 - p^\dagger(p)$.

The random walk that results is like an adjoint simulation in which all particles originate at $p_0$.

Our adjoint-mode estimators differ from the Albert estimator in the following aspects:

1. The Albert estimator assumes an absorbing Markov chain model for which appears the chain termination probability $p^\dagger(p_n)$, while ours uses a nonabsorbing chain model. Thus, the underlying Markov chain models are different. Our use of a nonabsorbing Markov chain model allows us to implement our approach of chain segmentation without the introduction of complicated, conditional termination probabilities.

2. Our objective is gathering several contributions to the different terms of the Neumann series of the solution, rather than single components of the solution at one or several points, as determined by the Albert estimator over a terminating chain.

3. The Albert estimator uses an underlying adjoint random walk and estimates over it in a forward manner. Three of our presented estimators have an underlying forward walk, over which they estimate either in a forward or an adjoint manner. Three other estimators that have an adjoint random walk over which they estimate either in a forward or adjoint manner have also been derived.

4. The idea of breaking up the chain into connected segments, and using the first collision source over these segments to obtain multiple contributions to each of the terms of the Neumann series at each collision point, has no equivalent in the Monte Carlo literature, to our best knowledge.

In Figs. A.2 and 2 the above discussion is displayed graphically, as well as the method of segmenting the chain and obtaining extra estimates of the terms of the Neumann series at each collision point, compared to those obtained over the generated chains without the application of our proposed estimators.

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REFERENCES


