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Transport-Constrained Extensions of Collision and Track Length Estimators for Solutions of Radiative Transport Problems

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Abstract

In this paper we develop novel extensions of collision and track length estimators for the complete space-angle solutions of radiative transport problems. We derive the relevant equations, prove that our new estimators are unbiased, and compare their performance with that of more conventional estimators. Such comparisons based on numerical solutions of simple one dimensional slab problems indicate the potential superiority of the new estimators for a wide variety of more general transport problems.

Keywords

Kernel density estimators; Radiative transport equations; Biased and unbiased estimators; Automated Monte Carlo algorithms

1. Introduction

In this paper we develop novel extensions of collision and track length estimators for the complete space-angle solutions of radiative transport problems. We derive the relevant equations, prove that our new estimators are unbiased, and compare their performance with that of kernel density estimators. The new estimators can be seen as expected value, or next event, estimators that incorporate both the scattering phase function and the normal exponential transport along a fixed ray. It is through the addition of angular information that the estimators obtain their increased computational power, especially for problems whose solutions are not well represented as isotropic. Our numerical evidence for this improvement is demonstrated here based on numerical solutions of simple one dimensional slab problems. More extensive numerical studies are currently underway and will be reported separately.

2. Extended Collision and Track Length Estimators

We have previously [6, 7, 8, 9, 10, 11, 12, 13, 14, 15] developed various adaptive Monte Carlo (MC) algorithms for estimating global solutions of radiative transport problems much faster than with conventional non-adaptive MC simulation. Our first such algorithm

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produces unbiased estimates of *truncated* expansions of the RTE solution in an infinite set of basis functions. In [21] this is called the *functional expansion tally* (FET) method. The output of such algorithms is a finite set of expansion coefficients from which a globally defined approximate solution can be reconstructed. We have shown that these adaptive algorithms converge *geometrically* (i.e., exponentially fast), producing very accurate solutions in low dimensions, but their performance degrades as the number of phase space variables increases because of the sheer number of expansion coefficients needed for accurate solution representations in some cases. An additional drawback is that such functional expansions converge very slowly for some problems and rapidly for others, and the user has no obvious way to determine in advance how many coefficients are needed in each independent variable to achieve the requisite accuracy. Technically speaking, these first generation (G1) adaptive methods are biased, the bias being determined by the number of expansion coefficients selected in each variable. Because of these limitations, we developed another strategy that represents the RTE solution as a histogram over a mesh (G2) that is coarse initially but which is then refined based on an information density function constructed from both the forward and the adjoint RTE solutions (G3) [13, 16, 17]. Although the initial mesh is revised in an automated way using this strategy, it is still necessary to define an *initial* mesh decomposition, which makes this option problem-dependent as well. While the G2-G3 method is faster than G1 methods in general, neither of them produces a truly *automated global* RTE solution. For that we seek a method that relies on *no* mesh other than that imposed by the physics (i.e., as a result of material heterogeneities) and uses a theoretically unbiased estimator.

By analogy with classical methods for solving ordinary and partial differential equations, these earlier solution representation methods would be more effective if the representation were tied more closely to the specific RTE being solved, as would be the case, for example, if one could base the solution expansion on a spectral decomposition of the RTE problem. But, because of the huge diversity and complexity of possible RTE problems and their solutions as the input data is varied, such spectral characterizations pose difficult analytic obstacles and challenges to carry out.

Our new, extended collision and track length estimators estimate the RTE solution at *any* point of phase space as a sum over *all* the collisions of points of *every* random walk. This method gives rise to unbiased estimators for all sample sizes that are much richer in information content and more powerful than traditional MC estimators.

The most straightforward way to develop the new estimators is from the integral, not the integro-differential form, of the RTE. In [18] we describe the integral form of the RTE (time-independent and one-speed) for the collision density $\Psi(\mathbf{r}, \omega)$:

$$\Psi(\mathbf{r}, \omega) = \int_L \int K(\mathbf{r}', \omega' \rightarrow \mathbf{r}, \omega) \Psi(\mathbf{r}', \omega') d\omega' dl + S(\mathbf{r}, \omega) \quad (1)$$

where L is a ray starting from $\mathbf{r}$ along the direction $-\omega$ and terminating at an interface or boundary of the (spatial) region. Analytically, $L = \{\mathbf{r} - \omega l \mid 0 \leq l \leq R\}$ where R indicates the nearest interface or boundary along the direction $-\omega$ and where the kernel K is

$$K(\mathbf{r}', \omega' \rightarrow \mathbf{r}, \omega) = \mu_s(\mathbf{r}') p(\omega' \cdot \omega; \mathbf{r}) \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}')} \mu_t(\mathbf{r}' + s\omega) ds \right] \quad (2)$$

In (2) the functions $\mu_s(\mathbf{r})$ and $\mu_t(\mathbf{r})$ are respectively the scattering and the total attenuation coefficients and $p(\omega' \cdot \omega; \mathbf{r})$ is the single scattering phase function at $\mathbf{r}$; it is a pdf for transforming the unit direction vector ω' to ω at collisions at $\mathbf{r}$ that result in scattering. The source term in (1) is

$$S(\mathbf{r}, \omega) = \int_D Q(\mathbf{r}', \omega) T(\mathbf{r}' \rightarrow \mathbf{r}, \omega) d\mathbf{r}'. \quad (3)$$

where the function $Q(\mathbf{r}, \omega)$ is the physical source density function; it is essentially the characteristic function that describes the locations and angular apertures of the instruments that produce the sources of radiation. The function T is an exponential

$$T(\mathbf{r}' \rightarrow \mathbf{r}, \omega) = \mu_t(\mathbf{r}') \exp \left[- \int_0^{\omega(\mathbf{r}-\mathbf{r}')} \mu_t(\mathbf{r}' + s\omega) ds \right] \quad (4)$$

that accounts for variation in the total attenuation coefficient along each track arising in the simulation. In many applications, the functions $\mu_t(\mathbf{r})$, $\mu_s(\mathbf{r})$ are assumed to be regionwise constant, thus simplifying the exponential term in (4). However, in the biomedical problems that provide our current focus, it is quite reasonable to imagine that these functions will even vary continuously when describing living tissue. In any event, we want to be certain that such descriptions can be accommodated by the methods we develop.

In biomedical problems there are 5 independent variables (3 for location and 2 for unit direction of travel). As well, the radiance $\Psi(\mathbf{r}, \omega)$ is determined from the collision density via

$$\Psi(\mathbf{r}, \omega) = \mu_t(\mathbf{r}) \Phi(\mathbf{r}, \omega). \quad (5)$$

for all $\mathbf{r}$ such that $\mu_t(\mathbf{r}) > 0$.

A number of random variables have been used in the past to provide unbiased estimates of linear functionals of the RTE solution such as

$$\int_D \int_{4\pi} g(\mathbf{r}, \omega) \Psi(\mathbf{r}, \omega) d\omega d\mathbf{r} \quad (6)$$

where g is a known function that describes one or more physical detectors. Those random variables most utilized in transport applications are probably the collision and the track length estimators. However, the scattering integrals appearing on the right hand side of (1) are themselves *functions* defined on the problem phase space that are closely related to the RTE solution itself. Our idea is to establish unbiased estimators for those functions (hence, the RTE solutions) that extend the “classical” collision and track length estimators to produce estimates of the entire RTE solution. We discuss these next.

To estimate the integral (6) where g is any function and Ψ is the solution of (1), the classical collision estimator [18] is defined as

$$\sum_{i=1}^{k(w)} g(\mathbf{r}_i, \omega_i) \quad (7)$$

where $w = (\mathbf{r}_1, \omega_1), \dots, (\mathbf{r}_{k(w)}, \omega_{k(w)})$ is a random walk consisting of collision points $(\mathbf{r}_i, \omega_i)$ and $k(w)$ is the final collision of w within the phase space geometry. With the same convention for designating the collision points of the random walk w , the generalized track length estimator [19] is

$$\sum_{i=1}^{k(w)+1} \int_{r_{i-1}}^{r_i} g(\mathbf{r}', \omega_{i-1}) d\mathbf{r}' \quad (8)$$

where the integral is over the individual tracks between $\mathbf{r}_{i-1}$ and $\mathbf{r}_i$ and $(\mathbf{r}_0, \omega_0)$ is the source location and direction and $(\mathbf{r}_{k(w)+1}, \omega_{k(w)+1})$ is the point at which the particle leaves the current region.

As we stated, the integral (6) defines a linear functional of the RTE solution; that is, it is a *number* for each choice of g . However, we may apply the estimators (7) and (8) to the functions that appear in the right hand side of (1) by simply applying them to *each fixed* $(\mathbf{r}, \omega) \in D \times 4$. If we adopt this perspective, the new extended collision estimator just involves summing evaluations of the kernel $\mathbf{K}(\mathbf{r}', \omega'; \mathbf{r}, \omega)$ over all collisions $(\mathbf{r}', \omega') = (\mathbf{r}_i, \omega_i)$, and the extended track length estimator involves summing integrals of the same kernel $\mathbf{K}$ over the tracks between collisions.

We illustrate the use of this idea by showing how such an extended collision estimator can be used to estimate the solution of (1).

Theorem 1

For each $(\mathbf{r}, \omega) \in D \times 4$ the random variable

$$\widehat{\Psi}_c(\mathbf{r}, \omega) = S(\mathbf{r}, \omega) + \sum_{i=1}^{k(w)} \mu_s(\mathbf{r}_i) p(\omega_i \cdot \omega; \mathbf{r}_i) \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_i)} \mu_t(\mathbf{r}_i + s\omega) ds \right] \quad (9)$$

provides an unbiased estimate of $\Psi(\mathbf{r}, \omega)$, where $(\mathbf{r}_1, \omega_1), (\mathbf{r}_2, \omega_2), \dots, (\mathbf{r}_{k(w)}, \omega_{k(w)})$ are the successive locations and directions of a random walk w .

Proof—From Equations (1) and (2), for each $(\mathbf{r}, \omega) \in D \times 4$, we see that the multiplier of in (1) is

$$\mathbf{K}(\mathbf{r}', \omega' \rightarrow \mathbf{r}, \omega) = \mu_s(\mathbf{r}') p(\omega' \cdot \omega; \mathbf{r}') \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}')} \mu_t(\mathbf{r}' + s\omega) ds \right].$$

Therefore, from (7), if we replace $(\mathbf{r}', \omega')$ by $(\mathbf{r}_i, \omega_i)$ in (2), we arrive at (9) making use of [18] Theorem 3.5.

From the definitions of the sample mean and variance it can be easily seen that, for W random walks, the variance of the W -sample mean of $\widehat{\Psi}_c(\mathbf{r}, \omega)$ can be calculated by

$$\begin{aligned} & \text{VAR}(\widehat{\Psi}_c(\mathbf{r}, \omega)) \\ &= \frac{1}{W-1} \left(\frac{1}{W} \sum_{w=1}^W \left(\sum_{i=1}^{k(w)} \mu_s(\mathbf{r}_i^w) p(\omega_i^w \cdot \omega; \mathbf{r}_i^w) \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_i^w)} \mu_t(\mathbf{r}_i^w + s\omega) ds \right] \right)^2 \right. \\ & \quad \left. - \left(\frac{1}{W} \sum_{w=1}^W \sum_{i=1}^{k(w)} \mu_s(\mathbf{r}_i^w) p(\omega_i^w \cdot \omega; \mathbf{r}_i^w) \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_i^w)} \mu_t(\mathbf{r}_i^w + s\omega) ds \right] \right)^2 \right). \end{aligned} \quad (10)$$

Similarly, an unbiased track length estimator for $(\mathbf{r}, \omega)$ follows in the same way:

$$\begin{aligned}
\widehat{\Psi}_{TL}(\mathbf{r}, \omega) &= S(\mathbf{r}, \omega) + \sum_{i=1}^{k(w)+1} \int_{r_{i-1}}^{r_i} \mathbf{K}(\mathbf{r}_i, \omega_i \rightarrow \mathbf{r}, \omega) dl \\
&= S(\mathbf{r}, \omega) + \sum_{i=1}^{k(w)+1} \int_0^{\omega_{i-1} \cdot (\mathbf{r}_i - \mathbf{r}_{i-1})} \mu_s(\mathbf{r}_{i-1} + l\omega_{i-1}) p(\omega_{i-1} \cdot \omega; \mathbf{r}_i) \\
&\quad \cdot \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_{i-1} - l\omega_{i-1})} \mu_t(\mathbf{r}_{i-1} + l\omega_{i-1} + s\omega) ds \right] dl
\end{aligned} \quad (11)$$

and its W -sample variance can be calculated by

$$\begin{aligned}
& \text{VAR}(\widehat{\Psi}_{TL}(\mathbf{r}, \omega)) \\
&= \frac{1}{W-1} \left(\frac{1}{W} \sum_{w=1}^W \left(\sum_{i=1}^{k(w)} \int_0^{\omega_{i-1}^w \cdot (\mathbf{r}_i^w - \mathbf{r}_{i-1}^w)} \mu_s(\mathbf{r}_{i-1}^w + l\omega_{i-1}^w) p(\omega_{i-1}^w \cdot \omega; \mathbf{r}_i^w) \right. \right. \\
&\quad \cdot \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_{i-1}^w - l\omega_{i-1}^w)} \mu_t(\mathbf{r}_{i-1}^w + l\omega_{i-1}^w + s\omega) ds \right] \Big)^2 \\
&\quad \left. - \left(\frac{1}{W} \sum_{w=1}^W \sum_{i=1}^{k(w)} \int_0^{\omega_{i-1}^w \cdot (\mathbf{r}_i^w - \mathbf{r}_{i-1}^w)} \mu_s(\mathbf{r}_{i-1}^w + l\omega_{i-1}^w) p(\omega_{i-1}^w \cdot \omega; \mathbf{r}_i^w) \right. \right. \\
&\quad \cdot \exp \left[- \int_0^{\omega \cdot (\mathbf{r} - \mathbf{r}_{i-1}^w - l\omega_{i-1}^w)} \mu_t(\mathbf{r}_{i-1}^w + l\omega_{i-1}^w + s\omega) ds \right] \Big) \Big).
\end{aligned} \quad (12)$$

These new estimators provide unbiased estimators of the RTE solution at any point and in any direction throughout the phase space. Examination of the explicit formulas (10) and (12) makes it clear that the sample variances are finite, unlike the variance of the simple point estimator which encounters a quadratic singularity as the collision point approaches the point at which the RTE solution is being estimated (see pp. 378ff of [25]). Each summand of both (10) and (12) is obviously finite (in fact, < 1) and the number of summands (= number of collisions) is finite with probability 1 because the governing RTE (1) allows only scattering and absorption upon collision: no multiplication.¹

These new estimators can be interpreted as generalized expected value, or next event estimators [18], pp. 101ff. For example, given $(\mathbf{r}, \omega) \in D \times 4\pi$, $\widehat{\Psi}_c(\mathbf{r}, \omega)$ is the sum of the (known) source function S and the sum over all collision points $(\mathbf{r}_j, \omega_j)$ of the conditional expected value that a particle, entering a collision at $\mathbf{r}_j$ in the direction ω_j will enter its *next* collision at $\mathbf{r}$ in direction ω . Figure 1 clarifies this idea and our interpretation of this generalized, or *extended*, next event estimator.

These extended collision and track length estimators treat *every* collision as a collision just prior to one at the phase space location and direction of the argument $(\mathbf{r}, \omega)$ of the collision density on the left-hand side of Eq. (1). This increase in information extracted from every random walk helps to explain the computational power of the new estimators. They have other advantages as well. First, they require the imposition of no mesh on the phase space other than that produced by the physical heterogeneities. Second, because the formula (9) can be evaluated for any $(\mathbf{r}, \omega)$, it provides the basis for plotting or otherwise displaying features of the RTE solution over any desired mesh, or of several such, based on a *single set of histories*. In Section 4 we will compare the performance of the new estimators with recently developed kernel density estimators, which they resemble in some ways.

N.B. For general heterogeneous RTE problems the new estimators can be evaluated by treating the integral that defines the exponent of the exponential term in (9) as a sum over the individual tracks from $\mathbf{r}_{i-1}$ to $\mathbf{r}_i$. In biomedical problems, it is often assumed, for example, that the tissue being modeled consists of a union of subvolumes each of which has

¹A more theoretical and general argument can be found in Section 3.3 of [18] based on the fact that the kernel K has norm < 1 .

constant optical properties. That is, the total attenuation function $\mu_t(\mathbf{r})$ is regionwise constant. In that case, each track produces a contribution

$$\frac{1}{\mu_t} [1 - \exp(-\mu_t l)]$$

where l is the length of the individual track and μ_t is the (constant) value of $\mu_t(\mathbf{r})$ along the track.

For simplicity, in the illustrations below we consider the special case for which the physical phase space is homogeneous and $\mu_s(\mathbf{r}) = \mu_s$, $\mu_t(\mathbf{r}) = \mu_t$ and $p(\hat{\mathbf{r}}; \mathbf{r}_i) = p(\hat{\mathbf{r}})$. Then (9) simplifies to:

$$\widehat{\Psi}_c(\mathbf{r}, \omega) = S(\mathbf{r}, \omega) + \sum_{i=1}^{k(\omega)} \mu_s p(\omega_i \cdot \omega) \exp[-\mu_t |\omega \cdot (\mathbf{r} - \mathbf{r}_i)|] \quad (13)$$

To clarify the practical use of this new estimator, we apply it to a very simple model problem.

3. An Application to a Simple Problem

We apply the extended collision estimator to a simply described family of transport problems in a slab of finite thickness T which is infinite in extent in the other two dimensions. A source of intensity Q_0 is introduced at the left ($x = 0$) boundary of the slab and only forward scattering and absorption are permitted throughout the slab. The integral form of the governing RTE is

$$\Psi(x) = Q_0 \exp(-\mu_t x) + \int_0^T K(x, y) \Psi(y) dy, \quad 0 \leq x \leq T \quad (14)$$

where

$$K(x, y) = \begin{cases} \mu_s \exp(-\mu_t(x - y)) & 0 \leq y \leq x \leq T \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

The solution, $\Psi(x)$, is the expected density of radiation at x . The nondimensionalized solution of this family of problems is easily seen to be

$$\Psi(x) = Q_0 \exp[-(1 - B_1) B_2 \xi] \quad 0 \leq \xi = x/T \leq 1 \quad (16)$$

where dimensionless groupings of parameters are defined by:

$$B_1 = \frac{\mu_s}{\mu_t} \quad B_2 = T \cdot \mu_t \quad (17)$$

The ratio B_1 determines the relative amounts of scattering and absorption in the slab, while the product B_2 defines the optical thickness of the slab. Small values of B_1 and B_2 characterize easier problems; large values describe harder² ones.

²Large parameter choices either result in the need to sample very many collisions per random walk to provide reliable solution estimates (large B_1) or require random walks to penetrate very large amounts of slab material (large B_2).

Our immediate goal is to specialize the estimator (13) to this particular simple family of problems, assuming for the present that the slab is homogeneous. Assume that each analog history w is described by the locations $w = (x_0 = 0, x_1, \dots, x_{k(w)})$ where, according to our notational convention that $k(w)$ indexes the final collision point *inside the slab*, either $x_{k(w)+1} > T$ or the history terminates through absorption at $x_{k(w)}$. The formula (13) reduces to

$$\widehat{\Psi}_c(x) = Q_0 \exp(-\mu_t x) + \sum_{i=1}^{k(w)} K(x, x_i) \quad (18)$$

where according to (15), the summands in the second term vanish for $x < x_i$.

To use this estimator, we would generate W random walks and store the locations x_i in a database. Then, to estimate the solution at *any* point x , we retrieve the x_i and evaluate the estimator defined in (18) at x . Suppose for example that we choose the following input data for problem (14):

$$\begin{aligned} Q_0 &= 1, \\ \mu_t &= 1, \\ \mu_s &= 0.25 \\ T &= 5, \end{aligned}$$

for which the exact solution is

$$\Psi(x) = \exp[-0.75x] \quad 0 \leq x/5 \leq 1.$$

To illustrate, we generated $W = 20$ random walks for this problem and produced the following table of collision points indicating the collision locations in the interval $[0, T = 5]$ for each of the 20 random walks:

W	collision 1	collision 2	collision 3
1	0.0002583	1.264	
2	1.462		
3	0.04345		
4	0.6161		
5	0.2745		
6	1.153		
7	0.6546	1.398	
8	1.507		
9	1.098	1.156	
10	0.1072		
11	0.6959		
12	1.702		
13	2.142	2.576	
14	0.4508		

W	collision 1	collision 2	collision 3
15	2.307		
16	2.227	2.916	4.157
17	0.6026	1.833	
18	1.482		
19	1.961		
20	0.3755	1.195	2.362

For any x in this interval, the formula (18) yields

$$\widehat{\Psi}(x) = \exp(-x) + \frac{1}{20} \sum_{i=1}^{k(w)} K(x, x_i).$$

The sum produces an exponential term for each value of $x_i < x$ and contributes 0 otherwise since the random walk can reach x from x_i only if $x_i < x$.

Figure 2(a) displays both the estimated and the exact solution values at the points $x = 0, 1, 2, 3, 4, 5$. *Without generating any new collision points*, we can estimate the solution at any different set of points. For example, Figure 2(b) compares the exact and the estimated solutions at 50 equally spaced points in the same interval. Notice that even though we generated only 20 random walks, the solution is remarkably well represented because *all* of the collisions play a role in the final estimate at *every* point. With only 20 random walks that make only 29 collisions in all, it is not surprising to see some fluctuations in the estimated solution.

This example illustrates one of the major advantages of the extended collision and track length estimators. The grid used to compute and plot the values of (9) can be chosen *after* the database of collisions is generated, and is completely independent of the locations and directions that make up that database. Therefore, post-processing the database of collision points from a single simulation can produce many estimating curves using the estimator (18). For example, we can use this flexibility either to capture the full solution everywhere throughout the phase space, or we can use it to focus attention on specific regions that may have special importance for the study we are conducting. Before testing this new estimator further, we discuss how kernel density estimators can be used for these RTE applications.

4. Kernel Density Estimators for RTEs

Density estimation is a statistical technique that constructs an estimate of an unknown probability density function (pdf) $f(x)$ from a set $X_1, \dots, X_n$ of observations of the underlying random variable [1]. This means that the observations form a set of n iid random variables each of which has the density $f(x)$. One very popular method for implementing density estimation - kernel density estimation - estimates the pdf as a sum of simple functions that are centered (usually symmetrically) at each sample point and decay away from each sample. In the single variable case one can write this estimate as

$$\widehat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^n k\left(\frac{x - X_i}{h}\right) \quad (19)$$

In (19), the function k is called the *kernel*, and it is usually chosen to be a pdf itself, which makes $\widehat{f}_h(x)$ a pdf, too. The parameter h is called the *smoothing parameter* and it controls the spread of the kernel about each data point.

Perhaps the oldest kde method is the histogram, which is defined by replacing k in (19) by the function

$$k(x) = \begin{cases} 1 & \text{if } |x| \leq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

and places a rectangle of height 1 and width h centered at each X_i . The resulting histogram pdf produces the familiar staircase cumulative distribution function with jumps at each sample point.

Kernel density estimation is a non-parametric method (i.e., no assumptions are made about the unknown underlying pdf), and the kernel can be chosen in a variety of ways: for example, as a standard Gaussian density

$$k_G(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \quad (20)$$

if x ranges over the entire real line, or as the Epanechnikov density

$$k_E(x) = \begin{cases} 6\left(\frac{1}{4} - x^2\right) & \text{if } x^2 < \frac{1}{4} \\ 0 & \text{otherwise} \end{cases} \quad (21)$$

or in various other ways. The popularity of the kernel density estimation approach stems partly from the fact that it is relatively simple to apply and (with sufficient restrictions) to analyze and that it can be shown to be consistent; that is, one can prove that $\widehat{f}_h(x)$ converges to $f(x)$ as the number of samples n increases without limit, provided that the smoothing parameter h tends to 0 in such a way that the product hn tends to ∞ . This last requirement means roughly that there are sufficiently many samples within the support sets of the kernel as the smoothing parameter is reduced.

Kernel density estimation (kde) methods can be used to represent the solution of the radiative transport equation (RTE) in full generality by considering the solution as an unnormalized probability density function defined over the problem phase space, $\mathcal{P}$. This general approach has recently been discussed in [23] in connection with nuclear reactor applications, and has also been used by the image synthesis community [3] and applied within the film and animation industries to create photorealistic appearances via computation. When applying conventional kde in this context, it produces a biased estimator of the RTE solution that requires a good choice of one or more smoothing parameters and careful treatment of boundary and interface conditions to be effective. Much of the utility and accuracy of kdes is tied to careful choices of such smoothing parameters and treatment of boundary conditions, and there is now a sizeable research literature devoted to this topic [1, 4, 2, 5].

In this section we will formulate collision-based kernel density estimators for transport problems like those in [23]. In [18] it is shown that an appropriate sample space for RTE simulations is the set of all (analog) random walks w constructed by sampling from S to obtain the location and direction of the first collision, and using the kernel K of the integral RTE (1) repeatedly to obtain the locations and directions of all succeeding collisions. Each

random walk constructed in this manner consists of a sequence of collision points, $w = \{(\mathbf{r}_1, \omega_1), \dots, (\mathbf{r}_{k(w)}, \omega_{k(w)})\}$ where $\mathbf{r}_j \in \mathcal{R}^3$ is a 3-dimensional spatial vector and $\omega_j \in \mathcal{S}^2$ is a polar representation of vectors on the unit sphere. According to the measure-theoretic theory presented in [18], such random walks $w_1, \dots, w_W$ provide iid samples from a pdf that is characterized by the (normalized) solution of (1).

We continue to restrict our attention to the one-dimensional case here, but for the purpose of testing and comparing our algorithms' performances, we generalize the monodirectional slab transport problem discussed earlier to the bidirectional case. It is straightforward to test the same algorithms on higher dimensional transport problems. In one dimension the spatial vector $\mathbf{r}$ will become x , and the unit direction vector is a discrete vector with only two components that we designate by the integers 1 (left to right) and 2 (right to left). In this setting, a sample random walk is described by the $k(w)$ -tuple $\{(x_1, n_1), (x_2, n_2), \dots, (x_{k(w)}, n_{k(w)})\}$ where $n_j \in \{1, 2\}$.

This bidirectional slab transport problem can be modeled as a pair of coupled differential equations

$$\begin{cases} \frac{d\Psi_1}{dx} + \mu_t \Psi_1 = \mu_s (p_{11} \Psi_1 + p_{12} \Psi_2) + Q_1(x), & 0 < x \leq T, \\ -\frac{d\Psi_2}{dx} + \mu_t \Psi_2 = \mu_s (p_{21} \Psi_1 + p_{22} \Psi_2) + Q_2(x), & 0 \leq x < T, \\ \Psi_1(0) = Q_0, \Psi_2(T) = Q_T \end{cases} \quad (22)$$

where

$$\begin{aligned} Q_0, Q_T &\geq 0, \quad Q_1(x), Q_2(x) \geq 0, \\ \mu_t &\geq \mu_s \geq 0, \\ p_{11}, p_{12}, p_{21}, p_{22} &\geq 0 \\ p_{11} + p_{21} &= 1, \quad p_{12} + p_{22} = 1. \end{aligned} \quad (23)$$

The constants μ_s, μ_t describe the scattering and total attenuation coefficients, respectively, and p_{ij} is the probability of scattering from direction j to i , where $i = j = 1$ corresponds to motion from left to right in the slab while $i = j = 2$ corresponds to motion from right to left. The function Ψ_1 thus describes left-to-right-moving radiation and Ψ_2 describes right-to-left-moving radiation. Formulas for the solutions of such problems may be found, for example, in [20]. It is because we have exact solutions for this special system, which nevertheless provides valuable insights about higher dimensional applications, that we have often found it ideal for testing newly developed algorithms for solutions of RTEs.

The problem described by Equations (22), (23) can be converted to the system of coupled integral equations:

$$\begin{aligned} \Psi_1(x) &= \mu_s \left(p_{11} \int_0^x e^{-\mu_t(x-y)} \Psi_1(y) dy + p_{12} \int_0^x e^{-\mu_t(x-y)} \Psi_2(y) dy \right) \\ &\quad + Q_0 e^{-\mu_t x} + \int_0^x e^{-\mu_t(x-y)} Q_1(y) dy, \\ \Psi_2(x) &= \mu_s \left(p_{21} \int_x^T e^{-\mu_t(y-x)} \Psi_1(y) dy + p_{22} \int_x^T e^{-\mu_t(y-x)} \Psi_2(y) dy \right) \\ &\quad + Q_T e^{-\mu_t(T-x)} + \int_x^T e^{-\mu_t(T-y)} Q_2(y) dy, \end{aligned} \quad (24)$$

or

$$\begin{aligned} \Psi_1(x) &= \int_0^T K_{11}(x, y) \Psi_1(y) dy + \int_0^T K_{12}(x, y) \Psi_2(y) dy + S_1(x), \\ \Psi_2(x) &= \int_0^T K_{21}(x, y) \Psi_1(y) dy + \int_0^T K_{22}(x, y) \Psi_2(y) dy + S_2(x). \end{aligned} \quad (25)$$

where

$$\begin{aligned}
 K_{11}(x, y) &= \begin{cases} p_{11}\mu_s e^{-\mu_t(x-y)}, & \text{if } y \leq x, \\ 0, & \text{if } y > x, \end{cases} \\
 K_{12}(x, y) &= \begin{cases} p_{12}\mu_s e^{-\mu_t(x-y)}, & \text{if } y \leq x, \\ 0, & \text{if } y > x, \end{cases} \\
 K_{21}(x, y) &= \begin{cases} p_{21}\mu_s e^{-\mu_t(y-x)}, & \text{if } y \geq x, \\ 0, & \text{if } y < x, \end{cases} \\
 K_{22}(x, y) &= \begin{cases} p_{22}\mu_s e^{-\mu_t(y-x)}, & \text{if } y \geq x, \\ 0, & \text{if } y < x, \end{cases} \\
 S_1(x) &= Q_0 e^{-\mu_t x} + \int_0^x e^{-\mu_t(x-y)} Q_1(y) dy, \\
 S_2(x) &= Q_T e^{-\mu_t(T-x)} + \int_x^T e^{-\mu_t(T-y)} Q_2(y) dy.
 \end{aligned} \tag{26}$$

For this problem, the formula (9) reduces to a simpler form

$$\widehat{\Psi}_1(x) = S_1(x) + \sum_{i=1}^{k_1} (H(v_i) K_{11}(x, x_i) + H(-v_i) K_{12}(x, x_i)), \tag{27}$$

$$\widehat{\Psi}_2(x) = S_2(x) + \sum_{i=1}^{k_2} (H(v_i) K_{21}(x, x_i) + H(-v_i) K_{22}(x, x_i)), \tag{28}$$

where $v_i = \pm 1$ indicate the directions of motion ($v_i = 1$ meaning right-moving and $v_i = -1$ meaning left-moving) while

$$H(v) = \begin{cases} 1 & \text{if } |v| \geq 0 \\ 0 & \text{otherwise} \end{cases} \tag{29}$$

is a Heaviside step function. The subscripts indicate that $\widehat{\Psi}_1$ estimates Ψ_1 and $\widehat{\Psi}_2$ estimates Ψ_2 . The scalar collision density for this problem is estimated by adding together the two components of the vector collision density: $\widehat{\Psi}(x) = \widehat{\Psi}_1(x) + \widehat{\Psi}_2(x)$.

The variances of $\widehat{\Psi}_1(x)$ and $\widehat{\Psi}_2(x)$ at a point x can be calculated easily from (10) (for W random walks)

$$\begin{aligned}
 \text{Var}[\widehat{\Psi}_1(x)] &= \frac{1}{W-1} \left(\frac{1}{W} \sum_{i=1}^W \left(\sum_{j=1}^{k_w} (H(v_j^w) K_{11}(x, x_i^w) + H(-v_j^w) K_{12}(x, x_i^w)) \right) \right)^2 \\
 &= \left(\frac{1}{W} \sum_{w=1}^W \sum_{i=1}^{k_w} (H(v_i^w) K_{11}(x, x_i^w) + H(-v_i^w) K_{12}(x, x_i^w)) \right)^2, \\
 \text{Var}[\widehat{\Psi}_2(x)] &= \frac{1}{W-1} \left(\frac{1}{W} \sum_{i=1}^W \left(\sum_{j=1}^{k_w} (H(v_j^w) K_{21}(x, x_i^w) + H(-v_j^w) K_{22}(x, x_i^w)) \right) \right)^2 \\
 &= \left(\frac{1}{W} \sum_{w=1}^W \sum_{i=1}^{k_w} (H(v_i^w) K_{21}(x, x_i^w) + H(-v_i^w) K_{22}(x, x_i^w)) \right)^2.
 \end{aligned}$$

We will use the kde formula (19) to define our biased kdes for RTE problems. To define a suitable kernel k for use in (19), we select a nonnegative function $k(x)$ with finite support, e.g., in $[-1/2, 1/2]$, and we assume that

$$\int_{-1/2}^{1/2} k(x) dx = 1.$$

so that $k(x)$ is a pdf. Since each component of the solution vector $\Psi(x)$ is a scalar function, we will use the same kernel $k(x)$ for both components and we will from this point on drop the vector notation. We next define the local pdf

$$k_h(x) = \frac{1}{h} k\left(\frac{x}{h}\right)$$

where h is again a suitably chosen smoothing parameter. If

$\{(x_1^w, n_1^w), (x_2^w, n_2^w), \dots, (x_{k(w)}^w, n_{k(w)}^w)\}_{w=1}^W$ are the sample collision points, a collision-based kernel density estimator for the collision density $\Psi = \{\Psi_1(x), \Psi_2(x)\}$ can be defined for each component of the solution by mimicking (19):

$$\hat{\Psi}_h(x) = \frac{1}{W} \sum_{w=1}^W \sum_{i=1}^{k(w)} k_h(x - x_i^w), \quad (29)$$

The smoothing parameter h can be chosen arbitrarily, but it will affect the performance of the solutions estimated by (29). As is done frequently in the literature, we adopt the mean integrated square error (*MISE*) to measure the quality of the estimate (see [1]):

$$\begin{aligned} MISE &= E \int (\tilde{\Psi}_h(x) - \Psi(x))^2 dx \\ &= \int (E \tilde{\Psi}_h(x) - \Psi(x))^2 dx + \int \text{Var}[\tilde{\Psi}_h(x)] dx \end{aligned} \quad (30)$$

The first term of the right hand side of (30) is the integral of the squared bias, while the second term is the integrated variance. The bias tends to 0 as the smoothing parameter h tends to 0, while for fixed h , the variance tends to 0 as the number W of random walks tends to ∞ . In other words, we want to reduce h and increase W in order to reduce the *MISE* but we also want to ensure that the product hW as $W \rightarrow \infty$ and $h \rightarrow 0$. This suggests that there will exist an optimal smoothing parameter, h_{opt} that minimizes the *MISE*. According to [1], when the function $\Psi(x)$ to be estimated has an integrable second derivative, the optimal smoothing parameter h_{opt} can be determined roughly by the formula

$$h_{opt} = k_2^{-2/5} \left(\int k^2(x) dx \right)^{1/5} \left(\int \Psi''(x)^2 dx \right)^{-1/5} W^{-1/5} \quad (31)$$

where $\Psi''(x)$ is the second derivative of $\Psi(x)$, W is the total number of samples and

$$k_2 = \int x^2 k(x) dx. \quad (32)$$

Of course, in (31) the function $\Psi(x)$ is the normalized RTE solution we want to determine and is unknown. Because of this, conventional practice [1] is to evaluate the formula (31) for h_{opt} by replacing the solution $\Psi(x)$ in (31) by some standard density $\phi(x)$, such as the Gaussian density with variance σ^2 . When this is done, (31) results in

$$\begin{aligned}
 h_{opt} &= (4\pi)^{-1/10} \frac{3}{8} \pi^{-1/2} W^{-1/5} \\
 &= \frac{4}{3}^{1/5} \sigma W^{-1/5} \\
 &= 1.06 \sigma W^{-1/5}.
 \end{aligned} \tag{33}$$

Notice that both (31) and (33) are of order $W^{-1/5}$ so it is only the constants that multiply this term that are affected by the choice of the function $\varphi(x)$ used to determine h_{opt} in (31).

We next apply both the biased kernels and the extended next-event (ENE) estimator to the bidirectional slab transport problem. The formulas (29) applied to each component of $\tilde{\Psi}$ for the bidirectional slab problem become

$$\tilde{\Psi}_1(x) = \sum_{i=1}^{k(w)} H(v_i) \frac{1}{h} k\left(\frac{x-x_i}{h}\right), \tag{34}$$

$$\tilde{\Psi}_2(x) = \sum_{i=1}^{k(w)} H(-v_i) \frac{1}{h} k\left(\frac{x-x_i}{h}\right) \tag{35}$$

which we will implement for both the Epanechnikov kernel as defined by (21) and the histogram kernel defined by

$$k_h(x) = \begin{cases} 1 & \text{if } |x| < \frac{1}{2} \\ 0 & \text{otherwise} \end{cases} \tag{36}$$

Eq. (33) is used to determine the optimal smoothing parameter h_{opt} , where the sample standard deviation σ is estimated from the W random walks that define the sample data.

To calculate k_2 and $\int k_2(x) dx$ for the Epanechnikov kernel, we obtain

$$h_{opt} = 20^{2/5} \left(\frac{6}{5}\right)^{1/5} 2^{1/5} \sigma W^{-1/5} = 960^{1/5} \sigma W^{-1/5}. \tag{37}$$

and for the histogram kernel, we obtain

$$h_{opt} = 12^{2/5} 2^{1/5} \sigma W^{-1/5} = 288^{1/5} \sigma W^{-1/5}. \tag{38}$$

Each of the formulas (37) and (38) is used in the following iterative way to produce a good smoothing parameter for the chosen kernel. We first pick an initial smoothing parameter $h_0 > 0$ arbitrarily (in our tests we chose a relatively large value, $h_0 = 10$), then we estimate the standard deviation σ_0 by generating W random walks and applying the appropriate kernel density estimator to estimate the solutions of (25) at any number n of points. We define the initial standard deviation σ_0 as the average of the standard deviations of the estimated solution at all of the points. Substituting this σ_0 into either (37) or (38) yields a new smoothing parameter h_1 . Using this new smoothing parameter we can solve (25) again and repeat the previous steps. Our numerical results show that this iterative process converges quickly (here we performed 7 such iterations) to a value of the smoothing parameter that we then use for our final simulation.

For our comparative numerical studies we chose input data that corresponds to a prototypical biomedical problem:

$$\begin{aligned}
T &= 100, \\
Q_0 &= 1, Q_T = 0, \quad Q_1(x), Q_2(x) \equiv 0, \\
\mu_t &= 1 \text{ and } \mu_s = 0.99, \\
p_{11} &= 0.975 \text{ and } p_{12} = 0.025 \\
p_{11} + p_{21} &= 1, \quad p_{12} + p_{22} = 1,
\end{aligned} \tag{39}$$

which represents a homogeneous 100 mean free path thick slab problem with a photon source of unit intensity at $x = 0$ and scattering that is very forward peaked (g = average cosine of scattering angle) = 0.95. We generated 2000 random walks and used their collision points to estimate each component of the solution at 2000 equally spaced grid points in $[0, 100]$. The experiment was performed on a 2.4 GHz computer and the run times, variances, efficiencies and *MISE* are indicated in the following table:

	ENE	Histogram	Epanechnikov
T = run time (sec)	351	1673	1673
σ^2 = Variance	0.58	11.83	11.39
Eff = Efficiency	4.93E-03	5.05E-05	5.25E-05
<i>MISE</i>	0.021	0.601	0.580

The table shows that the computational efficiency, defined as

$$Eff = \frac{1}{\sigma^2 T}$$

of the new ENE collision estimator is about 2 orders of magnitude greater than that of either biased density estimator, with the run time advantage accounting for roughly a factor of 5 and the rest of the gain is due to decreased variance. The inherent cost per history of the biased kernels is actually somewhat smaller than for the ENE estimator, but the overhead associated with iterating to find a good smoothing parameter for each biased kernel greatly magnifies their cost.

As for the smoothing parameters, the iterative processes defined by (37) and (38) produced the following optimal smoothing parameters for the histogram kernel and Epanechnikov kernel:

$$\begin{aligned}
\text{histogram } h_{opt} &= 0.045, \\
\text{Epanechnikov } h_{opt} &= 0.056,
\end{aligned}$$

The boundary at $x = 0$ can create an especially large bias for the histogram and Epanechnikov estimators unless some device is used to avoid overspill of these estimators close to that boundary. This causes the two biased estimators to underestimate the solution values near that point. This can be addressed in a number of ways [22]. We have chosen a simple technique to minimize this additional bias for this test by reducing the size of the smoothing parameter in the vicinity of the boundary. The fact that the histogram and Epanechnikov estimator have unit integral at each collision point means that a reduction in h increases the height of the pdf near the boundary and helps to overcome this problem. We

omit the details. The paper [22] provides a nice description of various other methods for handling boundary effects in problems with bounded sample spaces, as does [23].

Figure 3(a) shows the scalar flux $\tilde{\Psi}_1(x) + \tilde{\Psi}_2(x)$ obtained using the histogram and ENE collision estimator kernels plotted against the exact solution, while Figure 4(a) shows the Epanechnikov and ENE estimators for the same problem. Figures 3(b) and 4(b) show the same estimators with error bars based on their standard deviations at the same set of points. The advantages of the ENE estimator are obvious from these figures.

We also performed similar comparisons for a heterogeneous 1D problem. For this we chose input data drawn from [26] and [27]. They study a two-layer model (see Figs.1 and 4 of [26]) of cervical epithelial tissue, with a thin upper layer (thickness $0.3mm$) of epithelium and an infinite lower stromal layer. We represented this problem as a 3-layer problem with both the 2nd and 3rd layers representing stromal tissue having identical optical characteristics. We placed an interface between layers 2 and 3, and chose a thin ($0.3mm$) 2nd layer.

In Table 1 of [27] specific optical properties are given. In fact, the paper gives two sets of optical properties for two different wavelengths of light (450 nm and 650 nm.) To illustrate how the estimators compare for realistic models of tissue, we chose the data for the 650 nm. wavelength:

Source:	$Q_0=1, Q_T=0, \quad Q_1(x), Q_2(x) \equiv 0,$
total slab thickness:	$T=10,$
first layer:	$x \in [0, 0.3],$
second layer:	$x \in [0.3, 0.6],$
third layer:	$x \in [0.6, 10],$

First layer optical properties :

$$\mu_{t1} = 2.86, \mu_{s1}=2.74, g_1=0.95,$$

Second layer optical properties :

$$\mu_{t2} = 17.29, \mu_{s2}=17.2, g_2=0.88,$$

Third layer optical properties :

$$\mu_{t3} = 17.29, \mu_{s3}=17.2, g_3=0.88,$$

where μ_{ti}, μ_{si} denote total and scattering coefficients for the i th layer and, based on the the values of g_i 's, the $P_{ij}^{(l)}$'s (in equation (22)) can be decided by

$$\begin{aligned}
p_{11}^{(1)} &= p_{22}^{(1)} = (1+g_1)/2=0.975, \\
p_{12}^{(1)} &= p_{21}^{(1)} = (1-g_1)/2=0.025, \\
p_{11}^{(2)} &= p_{22}^{(2)} = (1+g_2)/2=0.94, \\
p_{12}^{(2)} &= p_{21}^{(2)} = (1-g_2)/2=0.06, \\
p_{11}^{(3)} &= p_{22}^{(3)} = (1+g_3)/2=0.94, \\
p_{12}^{(3)} &= p_{21}^{(3)} = (1+g_3)/2=0.06,
\end{aligned}$$

also designate the layer number. The problem modeled is a 10 mean free path thick 2-layer slab problem with a photon source of unit intensity at $x = 0$. Units of μ_b, μ_s are mm^{-1} . We generated 1000 random walks for each iteration of the smoothing parameter. Ten iterations were needed for the Histogram and Epanechnikov kernel density estimators to obtain stable values of the smoothing parameters. The database of collision points was used to estimate each component of the solution at 400 equally spaced grid points in $[0, 10]$. The experiment was performed on the same 2.4 GHz computer as for the homogeneous problem, and the run times, variances, efficiencies and *MISEs* are indicated in the following table:

	ENE	Histogram	Epanechnikov
$T = \text{run time (sec)}$	27	151.5	151.5
$\sigma^2 = \text{Variance}$	0.2746	0.8435	0.8194
$Eff = \text{Efficiency}$	0.1257	0.0078	0.0081
<i>MISE</i>	0.0089	0.0283	0.0274

For this heterogeneous model problem the computational efficiency of ENE is about 1.5 orders of magnitude greater than either kernel density estimator, and Figure 5 provides visual evidence of the superiority of the ENE estimator to either of the kernel density estimators. Figure 6(a) and 6(b) compare the standard deviations of the ENE with the Histogram estimator, and the ENE with the Epanechnikov estimator, respectively.

5. Summary, Conclusions and Future Work

We have developed novel extended collision and track length estimators for solving radiation transport problems. We have established their unbiasedness and compared their performance in simple 1-D slab problems with that of kernel density estimators, with which they share some desirable properties. For example, they provide complete space-angle solutions based on the generation of a single set of random walks which can be post-processed in order to obtain various local as well as global information. However, unlike the kernel density estimators, they are unbiased so they require no mesh to be imposed on the phase space nor any other “smoothing” parameters, nor do they require special treatment of boundaries or internal interfaces. Since the *MISE* of the new estimators consists only of the variance component, they should outperform kernel density estimators.

We chose kernel density estimators for our first comparison because in [23] they are shown to compare favorably with functional expansion tallies and the conventional histogram tally with respect to both accuracy and rate of convergence. The extended collision estimator provides about 2 orders of magnitude greater computational efficiency than either the histogram or Epanechnikov estimators for the one dimensional test problems studied here.

We believe that the use of the new estimators will significantly improve the performance of the adaptive Monte Carlo algorithms that we have developed earlier. Our immediate interest is to apply these new estimators to heterogeneous tissue problems in 5 independent variables. We plan next to test them in layered tissue problems that incorporate refractive index mismatches at the layer interfaces and boundaries of the tissue. We anticipate that the goal of achieving very fast and accurate adaptive Monte Carlo computational models for both forward and inverse transport problems using only modest computing resources (e.g., without the need for parallel processing) is realizable when we introduce these new estimators into our exponentially accelerated adaptive Monte Carlo algorithms.

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References

- [1]. Silverman, BW. Density Estimation for Statistics and Data Analysis. Chapman and Hall; 1986.
- [2]. Scott, DW. Multivariate Density Estimation: Theory, Practice and Visualization. Wiley Series in Probability and Mathematical Statistics, John Wiley and Sons, Inc.; 1990.
- [3]. Jensen, HW. Realistic Image Synthesis Using Photon Mapping. A.K. Peters; 2001.
- [4]. Devroye, L. A Course in Density Estimation. Vol. Progress in Probability and Statistics Volume 14. Birkhauser; 1987.
- [5]. Wand, MP.; Jones, MC. Kernel Smoothing. Chapman and Hall; 1995.
- [6]. Spanier, J. Geometrically Convergent Learning Algorithms for Global Solutions of Transport Problems. In: Niederreiter, H.; Spanier, J., editors. Monte Carlo and Quasi-Monte Carlo Methods 1998. Springer-Verlag; 1999. p. 98-113.
- [7]. Kong, R.; Spanier, J. Sequential Correlated Sampling Methods for Some Transport Problems. In: Niederreiter, H.; Spanier, J., editors. Monte Carlo and Quasi-Monte Carlo Methods 1998. Springer-Verlag; 1999. p. 238-251.
- [8]. Kong, R.; Spanier, J. Error Analysis of Sequential Monte Carlo Methods for Transport Problems. In: Niederreiter, H.; Spanier, J., editors. Monte Carlo and Quasi-Monte Carlo Methods 1998. Springer-Verlag; 1999. p. 252-272.
- [9]. Lai, Y.; Spanier, J. Adaptive Importance Sampling Algorithms for Transport Problems. In: Niederreiter, H.; Spanier, J., editors. Monte Carlo and Quasi-Monte Carlo Methods 1998. Springer-Verlag; 1999. p. 273-283.
- [10]. Hayakawa, Carole; Spanier, J. Comparison of Monte Carlo Algorithms for Obtaining Geometric Convergence for Model Transport Problems. In: Niederreiter, H.; Spanier, J., editors. Monte Carlo and Quasi-Monte Carlo Methods 1998. Springer-Verlag; 1999. p. 214-226.
- [11]. Spanier, J.; Kong, R. A New Adaptive Method for Geometric Convergence. In: Niederreiter, H., editor. Monte Carlo and Quasi-Monte Carlo Methods 2002. Springer-Verlag; 2004. p. 439-449.
- [12]. Kong R, Spanier J. A new proof of geometric convergence for general transport problems based on sequential correlated sampling methods. *J. Comp. Phys.* 2008; 227:9762–77.
- [13]. Kong R, Ambrose M, Spanier J. Efficient, Automated Monte Carlo Methods for Radiation Transport. *J. Comp. Phys.* 2008; 227:9463–9476.
- [14]. Kong R, Spanier J. Geometric convergence of second generation adaptive Monte Carlo algorithms for general transport problems based on correlated sampling. *Int. J. Pure and Appl. Math.* 2010; 59:435–455.

- [15]. Kong R, Spanier J. Geometric Convergence of Adaptive Monte Carlo Algorithms for Radiative Transport Problems Based on Importance Sampling. Nucl. Sci. Eng. Jul.2011 168:197–225.
- [16]. Hayakawa, CK.; Kong, R.; Spanier, J. Spatial/Angular Contribution Maps for Improved Adaptive Monte Carlo Algorithms. Monte Carlo and Quasi-Monte Carlo Methods. 2010. to appear
- [17]. Bhan, K.; Kong, R.; Spanier, J. Monte Carlo and Quasi-Monte Carlo Methods 2008. Springer-Verlag; 2009. Adaptive Monte Carlo Algorithms Applied to Heterogeneous Transport Problems; p. 209-225.
- [18]. Spanier, J.; Gelbard, EM. Monte Carlo Principles and Neutron Transport Problems. Addison-Wesley Pub.Co.; 1969. (reprinted by Dover Pubs., Inc., 2008)
- [19]. Spanier J. Monte Carlo Methods for Flux Expansion Solutions of Transport Problems. NSE. 1999; 133:73–79.
- [20]. Spanier J. An Analytic Approach to Variance Reduction. SIAM J. Appl. Math. 1970; 18:172–190.
- [21]. Griesheimer DP, Martin WR, Holloway JP. Convergence properties of Monte Carlo functional expansion tallies. J.Comp. Phys. 2006; 211:129–153.
- [22]. Jones MC. Simple boundary correction for kernel density estimation. Statistic. and Computing. 1993; 3:135–146.
- [23]. Banerjee K, Martin WR. Kernel Density Estimation Method for Monte Carlo Global Flux Tallies. Nucl. Sci. Eng. 2012; 170:234–250.
- [24]. Banerjee K, Martin WR. Monte Carlo Global Scalar Flux Estimation with Kernel Density Estimator. Trans. Amer. Nucl. Soc. 2008; 99:346–7.
- [25]. Lux, I.; Koblinger, L. Monte Carlo Particle Transport Methods: Neutron and Photon Calculations. CRC Press; 1991.
- [26]. Chang SK, Drezek R, Follen M, Richards-Kortum R. Analytical model to describe fluorescence spectra of normal and preneoplastic epithelial tissue: comparison with Monte Carlo simulations and clinical measurements. Journal of Biomedical Optics. May-Jun;2004 9(3):511–522. [PubMed: 15189089]
- [27]. Arifler D, Schwarz RA, Chang SK, Richards-Kortum R. Reflectance spectroscopy for diagnosis of epithelial precancer: model-based analysis of fiber-optic probe designs to resolve spectral information from epithelium and stroma. APPLIED OPTICS. Jul 10.2005 Vol. 44(No. 20)

Figure 1.

Representation of $\widehat{\Psi}_c(\underline{r}, \underline{\omega})$ (Eq. (9)) as an Extended Next Event Estimator. The contribution to the solution at $(\underline{r}, \underline{\omega})$ from a collision at $\underline{r}_i$ with entering direction $\underline{\omega}_i$ is computed as the product of the conditional expected density value of a change of direction from $\underline{\omega}_i$ to $\underline{\omega}$ at $\underline{r}_i$ and the probability of a next collision at $\underline{r}$ from transport to $\underline{r}$ in direction $\underline{\omega}$.

Figure 2. Comparison of the exact solution (black) with the transport estimates (red) based on 20 random walks. 2(a) at $x = 0, 1, 2, 3, 4, 5$ and 2(b) at 50 equally spaced points in $(0, 5)$

Figure 3.

3(a) Comparison of the exact solution (black), transport estimates (red) and histogram estimates (blue dashed) at 2,000 equally spaced points over a 100 mean free path slab of tissue-like material. 3(b) includes error bars based on sample standard deviations

Figure 4.

4(a) Comparison of the exact solution (black), transport estimates (red) and Epanechnikov estimates (blue dashed) at 2,000 equally spaced points over a 100 mean free path slab of tissue-like material at 2,000 equally spaced points. 4(b) includes error bars based on sample standard deviations

Figure 5.
Visual Comparison of the Three Methods

Figure 6.

6(a) Comparison of Error Bars of ENE estimates (red) and Epanechnikov estimates (green)

6(b) Comparison of Error Bars of ENE estimates (red) and Histogram estimates (blue)