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A Proof of the Asymptotic Variance of Estimators for Monte Carlo Source Iteration in the Thick Diffusion Limit

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Abstract

We prove a theorem relating the variance of estimators for Monte Carlo source iteration methods to a parameter which becomes infinitesimally small in an important physical regime that arises in radiative transfer. In our usage, "Monte Carlo source iteration" refers to Monte Carlo Boltzmann transport methods in which each Monte Carlo particle history includes no more than a single collision. One example of this approach is modeling the physics of multiple scattering by lagging the scattering source term and iterating until this term converges.

The theorem that we prove can be used to construct variance reduction techniques which improve the order of the estimator variance when solving a linear Boltzmann transport equation. This improvement enables Monte Carlo source iteration calculations that would otherwise require impractically large sample sizes to achieve practical estimator uncertainties. Our proof relies on the expression of a Monte Carlo estimator as an expected value of a function of random variables. The function is chosen so that its expectation is a functional corresponding to the desired physical quantity. We derive this expression using a characteristic equation for the Boltzmann transport problem. We believe that this is the first postulation of a theorem relating the asymptotic estimator variance to a limiting case parameter in an important physical regime for Boltzmann transport, and the first proof of such a theorem.

We highlight the importance of the theorem with an example from the development of a linear transport method in which the authors of a publication describing the method used the theorem to design a variance reduction technique that improved the uncertainty of their solution by a factor of about 500 for a proxy problem from radiative transfer that contains both optically-thick and optically-thin material.

Keywords: Monte Carlo, Variance Reduction, Thick Diffusion Limit

1. Introduction

It is not uncommon to encounter substantial statistical variation when using Monte Carlo to compute the solution of a Boltzmann transport equation. This variation, or noise, can degrade solution quality enough that the Monte Carlo estimators become useless. The estimator uncertainty can be systematically reduced through sample augmentation, but the sample size required for an acceptable solution estimate may be impractical. Techniques that reduce the estimator variance also reduce the estimator uncertainty, which is proportional to the variance. The variance of a function of random variables f is,

$$\mathrm{Var}[f] = E[f^2] - (E[f])^2 \,, \tag{1}$$

where $E[\cdot]$ is the expectation, or expected value. Equation (1) shows that computing the variance requires the definition of f and the expectation, which is the first moment of f about the origin over its support.

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The Monte Carlo simulation procedure can be viewed as defining f, generating random variates of f, then averaging the variates. If $\mathrm{Var}[f]$ is too large, then Monte Carlo may be too expensive to solve the problem.

Asymptotic analysis is a technique that can be used to study how a numerical method behaves as an asymptotic analysis parameter approaches a particular limit. If a calculation which exercises the physical regime associated with the limiting case produces a noisy Monte Carlo estimator, then the estimator variance may have an undesirable dependence on the asymptotic analysis parameter. In the worst case, the estimator variance approaches infinity as the asymptotic analysis parameter approaches its limit. In the best case, the estimator variance approaches zero. If the limiting case is important to the application, then the difference between the best case and the worst case is the difference between a useful Monte Carlo method and a useless one. The theorem that we prove is a useful mathematical tool for this exact scenario.

In that sense, the theorem can be used as a powerful tool for designing variance reduction techniques. Variance reduction is an algorithmic development process aimed at improving Monte Carlo methods by reducing the variance of a Monte Carlo estimator. Modifying the Monte Carlo method to compute an estimator which has a variance that approaches zero in the limiting case would provide a substantial improvement: zero variance instead of infinite variance in the limit. Providing a proof of the theorem gives confidence that the empirical results (variance estimates) will match the theoretical result (analytic variances) when the number of samples is sufficiently large.

Our proof relies on the expression of a Monte Carlo estimator as an expected value of a function of random variables. This is a perspective which often appears in descriptions of Monte Carlo mathematics for Boltzmann transport, such as the textbooks by Spanier and Gelbard [1] and Lux and Koblinger [2]. Both texts present the collision density equation, the Fredholm integral equation of the second kind, and the Neumann series expansion, which the authors use in their analysis of multi-collision Monte Carlo. Our presentation is simplified by the restriction that the Monte Carlo particles can collide no more than once, though we do not impose any limit on the number of collisions undergone by physical particles. We achieve this by handling the physics of multiple collisions using source iteration, which lags the scattering source in order to avoid simulating scattering events in the Monte Carlo particle histories. Lagging the scattering source is uncommon in Monte Carlo methods but is essential for deterministic methods, where source iteration avoids forming and storing the transport operator [3].

The theorem that we prove relates the variance defined in eq. (1) to an asymptotic analysis parameter which becomes infinitesimally small in an important physical regime that arises in radiative transfer. We describe the regime in section 2, as well as some background information on the linear Boltzmann transport equation that we consider, before ending the section with a statement of the theorem. In section 3, we prove the theorem and discuss some limitations of the proof. In section 4, we provide an example of how the theorem can be applied to convert a method with a variance that limits to infinity into one that limits to zero. This resulted in an improvement in the uncertainty of a Monte Carlo estimator of the angle integrated intensity by a factor of about 500 for a proxy problem from radiative transfer that contains both optically-thick and optically-thin material. We conclude with a summary in section 5.

2. Statement of the Theorem

A statement of the theorem requires some background information on the Boltzmann transport problem under consideration. We provide this background information first, before finishing this section with the statement of the theorem. The Boltzmann transport problem that we consider is,

$$\mathbf{\Omega} \cdot \nabla \psi + \sigma_t \psi = Q \,, \tag{2a}$$

where $\mathbf{\Omega} \in \mathbb{R}^3$ is the unit direction vector, ψ is the radiation intensity, σ_t is the total material opacity, and Q is the total source function. Equation (2a) is subject to an inflow boundary condition, which defines the radiation intensity on the domain boundary in the hemisphere of directions that point into the domain at a given location on the domain boundary surface,

$$\psi(\mathbf{x}, \mathbf{\Omega}) = \psi_{\mathrm{inc}}(\mathbf{x}, \mathbf{\Omega}) \,, \quad \mathbf{x} \in \partial\mathcal{D} \text{ and } \mathbf{\Omega} \cdot \mathbf{n} < 0 \,, \tag{2b}$$

where $\mathbf{x} \in \mathbb{R}^3$ is the spatial position coordinate, ψ_{inc} is the inflow source function, $\partial\mathcal{D}$ is the domain boundary, and $\mathbf{n}$ is the outward facing unit normal vector on the domain boundary surface. To model a problem in which photons are scattered and emitted by electronic interactions with the material, we could define Q to be,

$$Q = \frac{\sigma_s}{4\pi} \int_{\mathbb{S}^2} \psi \, \mathrm{d}\Omega' + q \,, \tag{3}$$

where σ_s is the scattering opacity, $\mathbb{S}^2$ is the unit sphere, and q is an arbitrary source function with which to account for other ways that photons may enter phase space, such as photon emission from electronic de-excitations in the material.

A common approach for the Monte Carlo simulation of eq. (2a) with Q defined by eq. (3) involves simulating scattering events. In this approach, when a simulation particle undergoes a collision identified as a scattering event, it emerges with a new direction and a new frequency, both of which are chosen by pseudo-random sampling of the appropriate distributions. Multiple collisions can occur because scattering events do not terminate the particle history.

An alternative approach is to incorporate the contribution of the scattering source in the weight of the simulation particles. This necessitates an iteration to compute successive approximations of the integral in eq. (3), but it removes the possibility of multiple collisions. Without scattering events, simulation particles can only have at most one collision: a history with a single collision corresponds to a particle that was absorbed in the domain, and a history with no collisions corresponds to a particle that leaked through a vacuum boundary surface. The approach without scattering events is the one that we consider. Additionally, we choose to disregard frequency dependence as well as time dependence in the Boltzmann transport problem that we consider, hence why we write $\psi = \psi(\mathbf{x}, \mathbf{\Omega})$ instead of $\psi = \psi(\mathbf{x}, \mathbf{\Omega}, \nu, t)$.

The limiting case corresponding to the asymptotic analysis that we apply is called the thick diffusion limit (TDL) [4]. It is an optically-thick, highly-scattering transport regime characterized by an asymptotic analysis parameter $\epsilon \in (0, 1]$. The limit $\epsilon \to 0$, along with the following scalings of the transport problem data, define the TDL,

$$\sigma_t \leftarrow \sigma_t / \epsilon \,, \tag{4a}$$

$$\sigma_a \leftarrow \sigma_a \epsilon \,, \tag{4b}$$

$$q \leftarrow q\epsilon \,, \tag{4c}$$

where $\sigma_a = \sigma_t - \sigma_s$ is the absorption opacity. Thus, σ_s is $O(1/\epsilon)$ because $\sigma_s \leftarrow \sigma_t/\epsilon - \sigma_a\epsilon$ and $1/\epsilon \gg \epsilon$ when $\epsilon \to 0$. We can now state the theorem which connects the variance of Monte Carlo estimators for the transport eq. (2a) to the TDL parameter ϵ. The theorem is as follows:

Theorem 1. *Let Q be the total source function of a transport problem with the following form,*

$$\mathbf{\Omega} \cdot \nabla\psi + \sigma_t \psi = Q \,,$$

subject to the inflow boundary condition,

$$\psi(\mathbf{x}, \mathbf{\Omega}) = \psi_{inc}(\mathbf{x}, \mathbf{\Omega}) \,, \quad \mathbf{x} \in \partial\mathcal{D} \text{ and } \mathbf{\Omega} \cdot \mathbf{n} < 0 \,.$$

Let $\mathrm{Var}[\cdot]$ *be the variance of an estimator for some quantity in a weighted Monte Carlo particle simulation of this transport problem, such as the angle integrated intensity, and let ϵ be the thick diffusion scaling limit (TDL) parameter. Then* $\mathrm{Var}[\cdot]$ *is,*

$$O\left(\max\left\{ \mathrm{order}(Q)^2, \, \mathrm{order}(\psi_{inc})^2 \right\} \epsilon \right) ,$$

where $\mathrm{order}(Q)$ *and* $\mathrm{order}(\psi_{inc})$ *are the powers of ϵ which define the leading order term in the TDL scaling of Q and ψ_{inc}, respectively.*

3. Proof of the Theorem

Before presenting the proof, we provide an outline of the required steps. The proof we present pertains to a specific estimator and physical quantity—namely, the path length estimator of the angle integrated intensity. We denote this quantity as $\hat{\phi}$. After providing the outline, we present the proof. After the proof, we describe how to generalize it to accommodate a different estimator, such as a collision estimator or a surface crossing estimator, or a different quantity, such as the first angular moment or the second angular moment of the radiation intensity.

The outline of the proof is:

3.1 Derive the expectation for the Monte Carlo estimator $\hat{\phi}$ by completing the following substeps:

  3.1.1 Formally integrate the characteristic equation for eq. (2a) subject to the boundary condition eq. (2b) over all directions and over the volume enclosed by a single mesh element,

  3.1.2 Estimate the integral using Monte Carlo:
  - Change variables such that $s = 0$ defines a point on $\partial\mathcal{D}$ instead of $\mathcal{D}$,
  - Define sampling procedures for the volume and boundary sources by defining random variables, a joint probability density function, and a function of the random variables such that the expectation of the function is the integral that we want to compute,

3.2 Evaluate eq. (1) for $\text{Var}[f + g]$, where f and g are the functions of random variables which define the expectations that $\hat{\phi}$ approximates for the volume source and boundary source, respectively. Finally, simplify the expression by applying the TDL scaling eqs. (4a) to (4c) to arrive at the function of Q, ψ_{inc}, and ϵ listed in the statement of the theorem.

The proof is as follows:

Proof. This is the proof of theorem 1, which is divided into the parts described above.

3.1. Derive the expectation for the MC estimator $\hat{\phi}$

We begin by deriving the expectation for the MC estimator $\hat{\phi}$. The first step in this process is to formally integrate the characteristic equation over all directions and over the volume enclosed by a single mesh element.

3.1.1. Formally integrate the characteristic equation

The characteristic equation for eq. (2a) subject to the boundary condition given by eq. (2b) is,

$$\psi(\boldsymbol{r}, \boldsymbol{\Omega}) = e^{-\int_0^{s_0} \sigma_t(\boldsymbol{r}-\eta\boldsymbol{\Omega})\,\mathrm{d}\eta} \psi_{\text{inc}}(\boldsymbol{r} - s_0\boldsymbol{\Omega}, \boldsymbol{\Omega}) + \int_0^{s_0} e^{-\int_0^{s} \sigma_t(r-\eta\boldsymbol{\Omega})\,\mathrm{d}\eta} Q(\boldsymbol{r} - s\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{d}s\,, \tag{5}$$

where we changed notation for the spatial coordinate from $\mathbf{x}$ to $\boldsymbol{r} - s\boldsymbol{\Omega}$, the parameter s is the distance along the characteristic, and s_0 is the distance to the domain boundary in the $-\boldsymbol{\Omega}$ direction. To understand eq. (5), imagine placing a detector at the phase-space point $(\boldsymbol{r}, \boldsymbol{\Omega})$, shown as the black dot at $\boldsymbol{r}$ in fig. 1. The first term in eq. (5) represents particles emitted from the boundary $\partial\mathcal{D}$ in direction $\boldsymbol{\Omega}$ and exponentially attenuated before reaching the detector, while the second term represents particles emitted along s_0 with direction $\boldsymbol{\Omega}$ and similarly attenuated.

Integrate eq. (5) over the unit sphere, impose a mesh, and represent the quantity described by the angular integral as a piecewise constant function that is single-valued on each mesh element by averaging the angular integral over an arbitrary element K,

$$\begin{aligned}\frac{1}{\text{vol}(K)} \int_K \int_{\mathbb{S}^2} \psi(\boldsymbol{r}, \boldsymbol{\Omega})\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r} &= \frac{1}{\text{vol}(K)} \int_K \int_{\mathbb{S}^2} e^{-\int_0^{s_0} \sigma_t(\boldsymbol{r}-\eta\boldsymbol{\Omega})\,\mathrm{d}\eta} \psi_{\text{inc}}(\boldsymbol{r} - s_0\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r} \\ &+ \frac{1}{\text{vol}(K)} \int_K \int_{\mathbb{S}^2} \int_0^{s_0} e^{-\int_0^{s} \sigma_t(r-\eta\boldsymbol{\Omega})\,\mathrm{d}\eta} Q(\boldsymbol{r} - s\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{d}s\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}\,.\end{aligned} \tag{6}$$

Equation (6) is an integral equation for the classic piecewise constant Monte Carlo estimator of the angle integrated intensity. The left-hand side of eq. (6) can be approximated using Monte Carlo integration. If we knew ψ, then the Monte Carlo approximation of eq. (6) could be written as,

$$\frac{1}{\mathrm{vol}(K)} \int_K \int_{\mathbb{S}^2} \psi(\boldsymbol{r}, \boldsymbol{\Omega}) \,\mathrm{d}\Omega \,\mathrm{d}\boldsymbol{r} \approx \frac{4\pi}{N} \sum_{n=1}^{N} \psi(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}) \,, \tag{7}$$

where $\boldsymbol{r}^{(n)}$ and $\boldsymbol{\Omega}^{(n)}$ are random variates of uniform independent and identically distributed (iid) random variables in space and angle, respectively. We do not know ψ, so we use the right-hand side of eq. (6) to compute the sum in eq. (7).

3.1.2. Estimate the integral using Monte Carlo

In this part of the proof, we first change variables such that $s = 0$ defines a point on $\partial\mathcal{D}$ instead of $\mathcal{D}$, then we define sampling procedures for the volume and boundary sources by defining random variables, a joint probability density function, and a function of the random variables such that the expectation of the function is the integral that we want to compute.

Consider the change of variables,

$$\boldsymbol{r}' = \boldsymbol{r} - s\boldsymbol{\Omega}, \qquad \boldsymbol{\Omega}' = \Omega, \qquad s' = s \,. \tag{8}$$

Let $S \sim \mathrm{exponential}(\sigma_t(\boldsymbol{r}' + s\boldsymbol{\Omega}))$ be a random variable representing the distance traveled by a MC photon originating from the point $\boldsymbol{r}'$ and traveling in the direction $\boldsymbol{\Omega}$ before it collides with an electron in the matter. We refer to s as the “path length”. The probability density function for the path length s given a fixed position $\boldsymbol{r}'$ and direction $\boldsymbol{\Omega}$ is,

$$p_{\sigma_t}(s) = \sigma_t(\boldsymbol{r}' + s\boldsymbol{\Omega}) e^{-\int_0^s \sigma_t(\boldsymbol{r}' + \eta\boldsymbol{\Omega}) \,\mathrm{d}\eta} \,. \tag{9}$$

Using the notation $(\cdot\;; K)$ to emphasize the presence of element K, define the distance traveled in K as,

$$\tau(\boldsymbol{r}', \boldsymbol{\Omega}, s; K) = \begin{cases} 0 & s < s_1(\boldsymbol{r}', \boldsymbol{\Omega}; K) \,, \\ s - s_1(\boldsymbol{r}', \boldsymbol{\Omega}; K) & s_1(\boldsymbol{r}', \boldsymbol{\Omega}; K) \le s \le s_2(\boldsymbol{r}', \boldsymbol{\Omega}; K) \,, \\ s_2(\boldsymbol{r}', \boldsymbol{\Omega}; K) - s_1(\boldsymbol{r}', \boldsymbol{\Omega}; K) & s_2(\boldsymbol{r}', \boldsymbol{\Omega}; K) > s \,, \end{cases} \tag{10a}$$

where s_1 and s_2 are the distances to the entry point and exit points of K along $\boldsymbol{\Omega}$, respectively,

$$s_1(\boldsymbol{r}', \boldsymbol{\Omega}; K) = \min\{s \mid \boldsymbol{r}' + s\boldsymbol{\Omega} \in \partial K\} \,, \tag{10b}$$

$$s_2(\boldsymbol{r}', \boldsymbol{\Omega}; K) = \max\{s \mid \boldsymbol{r}' + s\boldsymbol{\Omega} \in \partial K\} \,. \tag{10c}$$

Figure 2 shows $\boldsymbol{r}'$ along with three possible absorption locations corresponding to three values of τ. Observe that $\boldsymbol{r}' \in \partial\mathcal{D}$. The final step in this change of variables $\boldsymbol{r} \to \boldsymbol{r}'$ is to relate the volume elements $\mathrm{d}\boldsymbol{r}$ and $\mathrm{d}\boldsymbol{r}'$.

Let $\mathbf{n}(\boldsymbol{r}')$ denote the surface normal vector at $\boldsymbol{r}' \in \partial\mathcal{D}$. Consider the volume, made by an infinitesimal area element $\mathrm{d}A$ on the boundary $\partial\mathcal{D}$ extruded by distance $\mathrm{d}s$ in direction $\boldsymbol{\Omega}$,

$$\{\boldsymbol{r}' + s\boldsymbol{\Omega} \,|\, \boldsymbol{r}' \in \mathrm{d}A \subset \partial\mathcal{D},\; s \in \hat{s} + \mathrm{d}s\} \,. \tag{11}$$

In two spatial dimensions, this volume is a function of the area of the parallelogram in $\mathrm{span}\{\mathbf{n}, \mathbf{n}^\perp\}$, where $\mathbf{n}^\perp$ is the unit vector perpendicular to the surface normal $\mathbf{n}$, formed from $\mathbf{n} \cdot \mathbf{n}^\perp = 0$ and shown in fig. 3. The volume is,

$$\mathrm{d}s \;\mathrm{d}A \,|\mathbf{n}^\perp \times \boldsymbol{\Omega}| = \mathrm{d}s \;\mathrm{d}A \left| \det \begin{pmatrix} n_2 & \Omega_1 \\ -n_1 & \Omega_2 \end{pmatrix} \right| \,, \tag{12}$$

where the subscripts denote the entry number of the value in the corresponding vector. Equation (12) simplifies to $\mathrm{d}s \;\mathrm{d}A \,|\boldsymbol{\Omega} \cdot \mathbf{n}|$. Also note that,

$$\int_0^s \sigma_t(\boldsymbol{r} - \eta\boldsymbol{\Omega}) \,\mathrm{d}\eta = \int_0^s \sigma_t(\boldsymbol{r}' + (s - \eta)\boldsymbol{\Omega}) \,\mathrm{d}\eta \,. \tag{13}$$

Letting $\tilde{\eta} = s - \eta$, so $\mathrm{d}\tilde{\eta} = -\,\mathrm{d}\eta$, we have,

$$\begin{aligned}\int_0^s \sigma_t(\boldsymbol{r}' + (s-\eta)\boldsymbol{\Omega})\,\mathrm{d}\eta &= -\int_s^0 \sigma_t(\boldsymbol{r}' + \tilde{\eta}\boldsymbol{\Omega})\,\mathrm{d}\tilde{\eta} \\ &= \int_0^s \sigma_t(\boldsymbol{r}' + \eta\boldsymbol{\Omega})\,\mathrm{d}\eta\,. \end{aligned} \tag{14}$$

Therefore, the integrand which is expressed in $\boldsymbol{r}$ coordinates,

$$e^{-\int_0^{s_0} \sigma_t(\boldsymbol{r}-\eta\boldsymbol{\Omega})\,\mathrm{d}\eta}\psi_{\mathrm{inc}}(\boldsymbol{r} - s_0\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{d}\boldsymbol{r} \tag{15}$$

can be equivalently represented as an integrand in $\boldsymbol{r}'$ coordinates,

$$e^{-\int_0^{s} \sigma_t(\boldsymbol{r}'+\eta\boldsymbol{\Omega})\,\mathrm{d}\eta}\psi_{\mathrm{inc}}(\boldsymbol{r}', \boldsymbol{\Omega})\,|\boldsymbol{\Omega}\cdot\mathbf{n}|\,\mathrm{d}s\,\mathrm{d}A\,. \tag{16}$$

The change of variables $\boldsymbol{r} \to \boldsymbol{r}'$ generates a factor of $|\boldsymbol{\Omega}\cdot\mathbf{n}|$ in the boundary surface integral because the infinitesimal volume element $\mathrm{d}\boldsymbol{r}$ is equal to $|\boldsymbol{\Omega}\cdot\mathbf{n}|\,\mathrm{d}s\,\mathrm{d}A$ in $\boldsymbol{r}'$ coordinates.

We proceed by considering the contribution of the volume source Q and the boundary source ψ_{inc} to $\hat{\phi}$ separately. First, the volume source.

Volume source contribution to $\hat{\phi}$

Let $\boldsymbol{R} \sim U(\mathcal{D})$, $\boldsymbol{\omega} \sim U(\mathbb{S}^2)$, and $S \sim \text{exponential}(\sigma_t(\boldsymbol{R}+s\boldsymbol{\omega}))$ be random variables representing the initial position, direction, and distance traveled by a MC photon from the volume source, respectively. Define the joint probability density function of $\boldsymbol{R}, \boldsymbol{\omega}$, and S as,

$$p(\boldsymbol{r}', \boldsymbol{\Omega}, s) = \frac{1}{\mathrm{vol}(\mathcal{D})}\frac{1}{4\pi}p_{\sigma_t}(\boldsymbol{r}', \boldsymbol{\Omega}, s)\,, \tag{17}$$

with domain $\mathcal{A} = \mathcal{D} \times \mathbb{S}^2 \times [0,\infty)$ and $p_{\sigma_t}(\boldsymbol{r}', \boldsymbol{\Omega}, s)$ defined in eq. (9). Define a function of the random variables $\boldsymbol{R}, \boldsymbol{\omega}$, and S representing the contribution of the volume source $Q(\boldsymbol{r}', \boldsymbol{\Omega})$ to the angle integrated intensity ϕ,

$$f(\boldsymbol{R}, \boldsymbol{\omega}, S) = 4\pi\;\mathrm{vol}(\mathcal{D})\,Q(\boldsymbol{r}', \boldsymbol{\Omega})\,\tau(\boldsymbol{r}', \boldsymbol{\Omega}, s; K)\,. \tag{18}$$

If $\psi_{\mathrm{inc}} = 0$ then eq. (6) can now be written in terms of the expectation of $f(\boldsymbol{R}, \boldsymbol{\omega}, S)$,

$$\frac{1}{\mathrm{vol}(K)}E\Big[f(\boldsymbol{R}, \boldsymbol{\omega}, S)\Big] = \frac{1}{\mathrm{vol}(K)}\int_{\mathcal{D}}\int_{\mathbb{S}^2}\int_0^\infty f(\boldsymbol{r}', \boldsymbol{\Omega}, s)\,p(\boldsymbol{r}', \boldsymbol{\Omega}, s)\,\mathrm{d}s\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}'\,, \tag{19}$$

where $p(\boldsymbol{r}', \boldsymbol{\Omega}, s)$ is the joint probability density function defined in eq. (17). The Monte Carlo approximation of the expectation in eq. (19) is,

$$E\Big[f(\boldsymbol{R}, \boldsymbol{\omega}, S)\Big] \approx \frac{1}{N}\sum_{n=1}^{N} f\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}, s^{(n)}\right)\,, \tag{20}$$

where $\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}, s^{(n)}\right)$, $n = 1, \ldots, N$, are random variates of the random variables $\boldsymbol{R}, \boldsymbol{\omega}$, and S. Substituting eq. (18) into eq. (20) gives,

$$\frac{1}{N}\sum_{n=1}^{N} f\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}, s^{(n)}\right) = \frac{4\pi\;\mathrm{vol}(\mathcal{D})}{N}\sum_{n=1}^{N} Q\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}\right)\tau\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}, s^{(n)}; K\right)\,. \tag{21}$$

Equation (21) is the contribution of the volume source to the $\hat{\phi}$ estimator. The sum in eq. (21) is over all N particles sourced in the volume $\mathcal{D}$. We can rewrite eq. (21) as a sum over all volume source particle paths

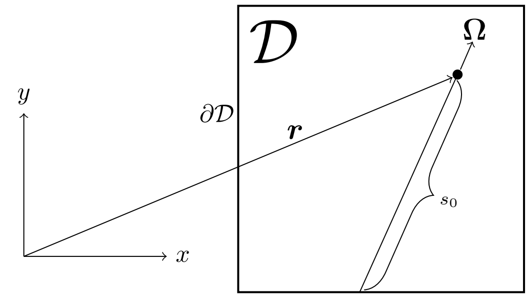


Figure 1: Distance to domain boundary $s_0(\boldsymbol{r})$.

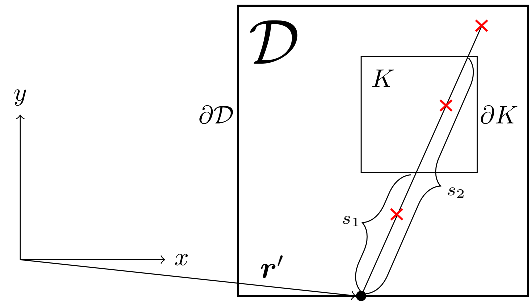
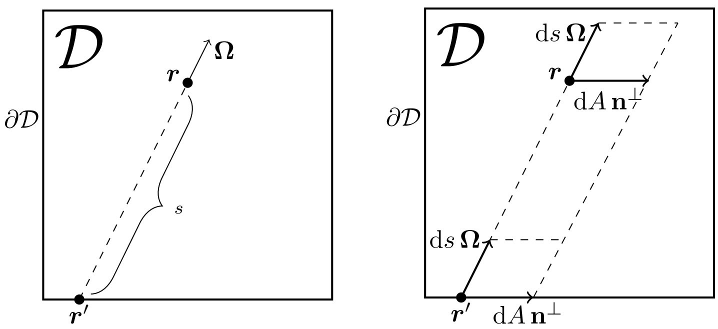


Figure 2: Distance to element entry $s_1(\boldsymbol{r}')$ and exit $s_2(\boldsymbol{r}')$ and three possible absorption locations marked by **X**'s along the path $\boldsymbol{r}' + s\boldsymbol{\Omega}$. Here, $\tau = 0$ for the **X** closest to $\boldsymbol{r}'$, $\tau = s - s_1$ for the middle **X**, and $\tau = s_2 - s_1$ for the far **X**.



(a) Change of variables.

(b) Volume scaling.

Figure 3: The change of variables $\boldsymbol{r} \to \boldsymbol{r}'$ generates a factor of $|\boldsymbol{\Omega}\cdot\mathbf{n}|$ in the boundary surface integral because $\mathrm{d}\boldsymbol{r} = |\boldsymbol{\Omega}\cdot\mathbf{n}|\,\mathrm{d}s\,\mathrm{d}A$.

traversed in some element K. Assume that volume source particle n traversed path i in element K and define its weight as,

$$w_i = \frac{4\pi \ \mathrm{vol}(\mathcal{D})}{N} Q\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}\right) . \tag{22}$$

Define the length of path i as,

$$d_i = \tau\left(\boldsymbol{r}^{(n)}, \boldsymbol{\Omega}^{(n)}, s^{(n)}; K\right) . \tag{23}$$

Equation (21) can now be rewritten as the sum over paths traversed by volume source particles in K,

$$\sum_{i=1} w_i d_i . \tag{24}$$

Multiplying eq. (24) by the inverse volume in front of the expectation in eq. (19) gives us our final result for the contribution of the volume source to the estimator $\hat{\phi}$ on K,

$$\frac{1}{\mathrm{vol}(K)} \sum_{i=1} w_i d_i . \tag{25}$$

Next, we consider the contribution of the boundary source ψ_{inc} to $\hat{\phi}$.

Boundary source contribution to $\hat{\phi}$

Let $\boldsymbol{R}_b \sim U(\partial\mathcal{D})$, $\boldsymbol{\omega}_h \sim U(\mathbb{S}_h^2)$, and $S_b \sim \mathrm{exponential}(\sigma_t(\boldsymbol{R}_b + s\boldsymbol{\omega}_h))$ be random variables representing the initial position, direction, and distance traveled by a MC photon from the boundary source, respectively, where $\mathbb{S}_h^2$ is all directions on the unit hemisphere defined by $\boldsymbol{\Omega}\cdot\mathbf{n} < 0$ at $\mathbf{x} \in \partial\mathcal{D}$. Define the joint probability density function of $\boldsymbol{R}_b, \boldsymbol{\omega}_h$, and S_b as,

$$\rho(\boldsymbol{r}', \boldsymbol{\Omega}, s) = \frac{1}{\mathrm{area}(\partial\mathcal{D})} \frac{1}{2\pi} p_{\sigma_t}(\boldsymbol{r}', \boldsymbol{\Omega}, s) , \tag{26}$$

with domain $\mathcal{B} = \partial\mathcal{D} \times \mathbb{S}_h^2 \times [0, \infty)$ and $p_{\sigma_t}(\boldsymbol{r}', \boldsymbol{\Omega}, s)$ defined in eq. (9). Define a function $g(\boldsymbol{R}_b, \boldsymbol{\omega}_h, S_b)$ of the random variables $\boldsymbol{R}_b, \boldsymbol{\omega}_h$, and S_b which represents the contribution of the boundary source $\psi_{\mathrm{inc}}(\boldsymbol{r}', \boldsymbol{\Omega})$ to the angle integrated intensity ϕ,

$$g(\boldsymbol{R}_b, \boldsymbol{\omega}_h, S) = 2\pi \ \mathrm{area}(\partial\mathcal{D}) \, \psi_{\mathrm{inc}}(\boldsymbol{r}', \boldsymbol{\Omega}) \, \tau(\boldsymbol{r}', \boldsymbol{\Omega}, s; K) . \tag{27}$$

If $Q = 0$ then Equation (6) can now be written in terms of the expectation of $g(\boldsymbol{R}_b, \boldsymbol{\omega}_h, S_b)$,

$$\frac{1}{\mathrm{vol}(K)} E\Big[g(\boldsymbol{R}_b, \boldsymbol{\omega}_h, S)\Big] = \frac{1}{\mathrm{vol}(K)} \int_{\partial\mathcal{D}} \int_{\boldsymbol{\Omega}\cdot\mathbf{n}<0} \int_0^\infty |\boldsymbol{\Omega}\cdot\mathbf{n}| \, g(\boldsymbol{r}', \boldsymbol{\Omega}, s) \, \rho(\boldsymbol{r}', \boldsymbol{\Omega}, s) \, \mathrm{d}s \, \mathrm{d}\Omega \, \mathrm{d}A , \tag{28}$$

where $\rho(\boldsymbol{r}', \boldsymbol{\Omega}, s)$ is the joint probability density function defined in eq. (26). The Monte Carlo approximation of the expectation in eq. (28) is,

$$E\Big[g(\boldsymbol{R}_b, \boldsymbol{\omega}_h, S)\Big] \approx \frac{1}{M} \sum_{m=1}^{M} g\left(\boldsymbol{r}_b^{(m)}, \boldsymbol{\Omega}_h^{(m)}, s_b^{(m)}\right) , \tag{29}$$

where $\left(\boldsymbol{r}_b^{(m)}, \boldsymbol{\Omega}_h^{(m)}, s_b^{(m)}\right)$, $m = 1, \ldots, M$, are random variates of the random variables $\boldsymbol{R}_b, \boldsymbol{\omega}_h$, and S_b. Substituting eq. (27) into eq. (29) gives,

$$\frac{1}{M} \sum_{m=1}^{M} g\left(\boldsymbol{r}_b^{(m)}, \boldsymbol{\Omega}_h^{(m)}, s_b^{(m)}\right) = \frac{2\pi \ \mathrm{area}(\partial\mathcal{D})}{M} \sum_{m=1}^{M} |\boldsymbol{\Omega}_h^{(m)} \cdot \mathbf{n}| \, \psi_{\mathrm{inc}}\left(\boldsymbol{r}_b^{(m)}, \boldsymbol{\Omega}_h^{(m)}\right) \tau\left(\boldsymbol{r}_b^{(m)}, \boldsymbol{\Omega}_h^{(m)}, s_b^{(m)}; K\right) . \tag{30}$$

Equation (30) is the contribution of the boundary source to the $\hat{\phi}$ estimator. The sum in eq. (30) is over all M particles sourced on the surface $\partial\mathcal{D}$. We can rewrite eq. (30) as a sum over all boundary source particle paths traversed in some element K. Assume that boundary source particle m traversed path j in element K and define its weight as,

$$w_j = \frac{2\pi \text{ area}(\partial\mathcal{D})}{M} |\mathbf{\Omega}_h^{(m)} \cdot \mathbf{n}| \, \psi_{\text{inc}} \left(\boldsymbol{r}_b^{(m)}, \mathbf{\Omega}_h^{(m)} \right) . \tag{31}$$

Define the length of path j as,

$$d_j = \tau \left(\boldsymbol{r}_b^{(m)}, \mathbf{\Omega}_h^{(m)}, s_b^{(m)}; K \right) . \tag{32}$$

Equation (30) can now be rewritten as the sum over paths traversed by boundary source particles in K,

$$\sum_{j=1} w_j d_j \, . \tag{33}$$

Multiplying eq. (33) by the inverse volume in front of the expectation in eq. (28) gives us our final result for the contribution of the boundary source to the estimator $\hat{\phi}$ on K,

$$\frac{1}{\text{vol}(K)} \sum_{j=1} w_j d_j \, . \tag{34}$$

The estimator $\hat{\phi}$ is the sum of eq. (25) and eq. (34).

Now that we have defined the expectation for the Monte Carlo estimator $\hat{\phi}$, we can evaluate eq. (1) for $\text{Var}[f+g]$, where f and g are the functions of random variables which define the expectations that $\hat{\phi}$ approximates for the volume source and boundary source, respectively.

3.2. *Evaluate* $\text{Var}[f+g]$ *and apply the TDL scaling*

The variance of a random variable, or a function of random variables, is the expectation of the square minus the square of the expectation, as shown in eq. (1) and rewritten here,

$$\text{Var}[f] = E[f^2] - (E[f])^2 \, . \tag{35}$$

Recall that $\hat{\phi}$ is the sum of eq. (25) and eq. (34). That is, $\hat{\phi}$ is the sum of contributions of particles originating from both the volume source Q and the boundary source ψ_{inc}. Thus, we must compute the variance of the sum of the functions of random variables which define the expectations,

$$\text{Var}[f+g] = \text{Var}[f] + \text{Var}[g] \, , \tag{36}$$

where we used $\text{Cov}[f, g] = 0$ because f and g are independent because they are functions of different independent random variables. We proceed by considering $\text{Var}[f]$ and $\text{Var}[g]$ separately. First, $\text{Var}[f]$.

Volume source contribution to $\text{Var}[f+g]$

Recalling eq. (19), which shows the expectation of f along with a volume factor, the expectation of f^2 is,

$$E[f^2] = \int_{\mathcal{D}} \int_{\mathbb{S}^2} \int_0^\infty f^2 p \, \mathrm{d}s \, \mathrm{d}\Omega \, \mathrm{d}\boldsymbol{r}' \, . \tag{37}$$

Considering only the integral along the particle path, we may substitute eqs. (17) and (18) for p and f, respectively, into eq. (37) and simplify to get,

$$\int_0^\infty f^2 p \, \mathrm{d}s = 4\pi \text{ vol}(\mathcal{D}) \, Q^2 \int_0^\infty \tau^2 p_{\sigma_t} \, \mathrm{d}s \, , \tag{38}$$

where p_{σ_t} and τ are defined by eqs. (9) and (10a), respectively. In a single material problem, the rate in the exponential probability density function is constant, and eq. (9) simplifies to,

$$p_{\sigma_t}(s) = \sigma_t e^{-\sigma_t s}\,. \tag{39}$$

Equation (39) in the TDL is,

$$p_{\sigma_t}(s) = \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s}\,, \tag{40}$$

where ϵ is the TDL scaling parameter. Now consider just the integral in eq. (38) without its coefficient. Substituting eq. (40) for p_{σ_t} and eq. (10a) for τ into the integral, and splitting the integral over $s \in [0,\infty)$ to three integrals over $[0,s_1)$, $[s_1,s_2)$, and $[s_2,\infty)$ gives,

$$\int_0^\infty \tau^2 p_{\sigma_t}\,\mathrm{d}s = \int_{s_1}^{s_2} (s-s_1)^2 \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s}\,\mathrm{d}s + (s_2-s_1)^2 \int_{s_2}^{\infty} \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s}\,\mathrm{d}s\,. \tag{41}$$

The second integral in eq. (41) is,

$$(s_2-s_1)^2 \int_{s_2}^{\infty} \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s}\,\mathrm{d}s = (s_2-s_1)^2 e^{-\frac{\sigma_t}{\epsilon} s_2}\,. \tag{42}$$

The first integral in eq. (41) may be computed using integration by parts twice. The result is,

$$\int_{s_1}^{s_2} (s-s_1)^2 \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s}\,\mathrm{d}s = 2\left(\frac{\epsilon}{\sigma_t}\right)^2 e^{-\frac{\sigma_t}{\epsilon} s_1} + \left\{-(s_2-s_1)^2 + 2s_1\left(\frac{\epsilon}{\sigma_t}\right) - 2s_2\left(\frac{\epsilon}{\sigma_t}\right) - 2\left(\frac{\epsilon}{\sigma_t}\right)^2\right\} e^{-\frac{\sigma_t}{\epsilon} s_2}\,. \tag{43}$$

We can now write eq. (41) as the sum of eqs. (42) and (43),

$$\int_0^\infty \tau^2 p_{\sigma_t}\,\mathrm{d}s = 2\left(\frac{\epsilon}{\sigma_t}\right)^2 e^{-\frac{\sigma_t}{\epsilon} s_1} + \left\{2s_1\left(\frac{\epsilon}{\sigma_t}\right) - 2s_2\left(\frac{\epsilon}{\sigma_t}\right) - 2\left(\frac{\epsilon}{\sigma_t}\right)^2\right\} e^{-\frac{\sigma_t}{\epsilon} s_2}\,. \tag{44}$$

Define a new random variable $\zeta_K^{(1)}$ equal to eq. (44),

$$\zeta_K^{(1)} = 2\left(\frac{\epsilon}{\sigma_t}\right)^2 e^{-\frac{\sigma_t}{\epsilon} s_1} + \left\{2s_1\left(\frac{\epsilon}{\sigma_t}\right) - 2s_2\left(\frac{\epsilon}{\sigma_t}\right) - 2\left(\frac{\epsilon}{\sigma_t}\right)^2\right\} e^{-\frac{\sigma_t}{\epsilon} s_2}\,. \tag{45}$$

We can label the terms and coefficients in eq. (45) to show the order of each term and coefficient in the TDL. Recall that in the TDL, $\epsilon^p < \epsilon^q$ for $p > q$, because $\epsilon \in (0,1]$. The terms in eq. (45) scale as,

$$\underbrace{\underbrace{2\left(\frac{\epsilon}{\sigma_t}\right)^2}_{O(\epsilon^2)} \underbrace{e^{-\frac{\sigma_t}{\epsilon} s_1}}_{O(1)}}_{O(\epsilon^2)} + \underbrace{\left(\underbrace{2s_1\left(\frac{\epsilon}{\sigma_t}\right)}_{O(\epsilon)} - \underbrace{2s_2\left(\frac{\epsilon}{\sigma_t}\right)}_{O(\epsilon)} - \underbrace{2\left(\frac{\epsilon}{\sigma_t}\right)^2}_{O(\epsilon^2)}\right) \underbrace{e^{-\frac{\sigma_t}{\epsilon} s_2}}_{O(1)}}_{O(\epsilon)}\,, \tag{46}$$

where the exponentials are bounded by 1 because $e^{-x} \in (0,1]$ for $x \geq 0$. Thus, $\zeta_K^{(1)}$ is $O(\epsilon)$.

Rewriting eq. (37) using eq. (38) with eq. (45) substituted, and then simplifying gives,

$$E[f^2] = 4\pi \ \mathrm{vol}(\mathcal{D}) \int_{\mathcal{D}} \int_{\mathbb{S}^2} Q^2\, \zeta_K^{(1)}\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}'\,. \tag{47}$$

We can label the terms in eq. (47) using the order of $\zeta_K^{(1)}$ determined in eq. (46) as follows,

$$\underbrace{\underbrace{4\pi\ \mathrm{vol}(\mathcal{D})}_{O(1)} \underbrace{\int_{\mathcal{D}} \int_{\mathbb{S}^2} \underbrace{Q^2}_{O(\mathrm{order}(Q)^2)} \underbrace{\zeta_K^{(1)}}_{O(\epsilon)} \,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}'}_{O(\mathrm{order}(Q)^2\ \epsilon)}}_{O(\mathrm{order}(Q)^2\ \epsilon)} \,. \tag{48}$$

Thus, $E[f^2]$ is $O(\mathrm{order}(Q)^2\ \epsilon)$, where $\mathrm{order}(Q)$ is the power of ϵ which defines the leading order term in the TDL scaling of Q

As shown by eq. (35), the variance is the difference of two terms, of which eq. (47) is only the first. The second is $(E[f])^2$, for which we must consider $E[f]$,

$$E[f] = \int_{\mathcal{D}} \int_{\mathbb{S}^2} \int_0^\infty f p \,\mathrm{d}s\,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}' \,. \tag{49}$$

The integral along the particle path is,

$$\int_0^\infty f p \,\mathrm{d}s = Q \int_0^\infty \tau p_{\sigma_t} \,\mathrm{d}s \,. \tag{50}$$

Substituting eq. (40) for p_{σ_t} and eq. (10a) for τ into the integral and splitting the integral into three as in eq. (41) gives,

$$\int_0^\infty \tau p_{\sigma_t} \,\mathrm{d}s = \int_{s_1}^{s_2} (s - s_1) \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s} \,\mathrm{d}s + (s_2 - s_1) \int_{s_2}^\infty \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s} \,\mathrm{d}s \,. \tag{51}$$

The second integral in eq. (51) is,

$$(s_2 - s_1) \int_{s_2}^\infty \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s} \,\mathrm{d}s = (s_2 - s_1) e^{-\frac{\sigma_t}{\epsilon} s_2} \,. \tag{52}$$

The first integral in eq. (51) may be computed using integration by parts. The result is,

$$\int_{s_1}^{s_2} (s - s_1) \frac{\sigma_t}{\epsilon} e^{-\frac{\sigma_t}{\epsilon} s} \,\mathrm{d}s = \left(s_1 - s_2 - \frac{\epsilon}{\sigma_t} \right) e^{-\frac{\sigma_t}{\epsilon} s_2} + \frac{\epsilon}{\sigma_t} e^{-\frac{\sigma_t}{\epsilon} s_1} \,. \tag{53}$$

We can now rewrite eq. (51) as the sum of eqs. (52) and (53),

$$\int_0^\infty \tau p_{\sigma_t} \,\mathrm{d}s = \frac{\epsilon}{\sigma_t} \left(e^{-\frac{\sigma_t}{\epsilon} s_1} - e^{-\frac{\sigma_t}{\epsilon} s_2} \right) \,. \tag{54}$$

Define a new random variable $\zeta_K^{(0)}$ equal to eq. (54),

$$\zeta_K^{(0)} = \frac{\epsilon}{\sigma_t} \left(e^{-\frac{\sigma_t}{\epsilon} s_1} - e^{-\frac{\sigma_t}{\epsilon} s_2} \right) \,. \tag{55}$$

We can label the terms and coefficients in eq. (55) to show the order of each term and coefficient. The terms in eq. (55) scale as,

$$\underbrace{\underbrace{\frac{\epsilon}{\sigma_t}}_{O(\epsilon)} \left(\underbrace{e^{-\frac{\sigma_t}{\epsilon} s_1}}_{O(1)} - \underbrace{e^{-\frac{\sigma_t}{\epsilon} s_2}}_{O(1)} \right)}_{O(\epsilon)} \,. \tag{56}$$

Thus, $\zeta_K^{(0)}$ is $O(\epsilon)$. Finally, we can rewrite eq. (49) using eq. (50) with eq. (55) substituted. After simplifying, the result is,

$$E[f] = \int_{\mathcal{D}} \int_{\mathbb{S}^2} Q\, \zeta_K^{(0)} \,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}' \,. \tag{57}$$

We can label the terms in eq. (57) using the order of $\zeta_K^{(0)}$ determined in eq. (56) as follows,

$$\underbrace{\int_{\mathcal{D}} \int_{\mathbb{S}^2} \underbrace{Q}_{O(\text{order}(Q))} \underbrace{\zeta_K^{(0)}}_{O(\epsilon)} \,\mathrm{d}\Omega\,\mathrm{d}\boldsymbol{r}'}_{O(\text{order}(Q)\ \epsilon)} \,. \tag{58}$$

Thus, $E[f]$ is $O(\text{order}(Q)\ \epsilon)$. We can now label the terms in the variance eq. (35), which scales as,

$$\mathrm{Var}[f] = \underbrace{\underbrace{E[f^2]}_{O(\text{order}(Q)^2\ \epsilon)} - \underbrace{(E[f])^2}_{O(\text{order}(Q)^2\ \epsilon^2)}}_{O(\text{order}(Q)^2\ \epsilon)} \,. \tag{59}$$

We now have the first term in eq. (36). For the second, $\mathrm{Var}[g]$, we must consider the boundary source.

Boundary source contribution to $\mathrm{Var}[f+g]$

Recall eq. (28), which shows the expectation of g along with a volume factor. The expectation of g^2 is,

$$E[g^2] = \int_{\partial\mathcal{D}} \int_{\boldsymbol{\Omega}\cdot\mathbf{n}<0} \int_0^{\infty} |\boldsymbol{\Omega}\cdot\mathbf{n}|\, g^2 \rho \,\mathrm{d}s\,\mathrm{d}\Omega\,\mathrm{d}A \,, \tag{60}$$

where ρ and g are defined by eqs. (26) and (27), respectively. If we apply the same procedure that we used to determine the order of $E[f^2]$ to eq. (60), we find that $E[g^2]$ is $O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)$. Similarly, applying the procedure that we used to determine the order of $E[f]$ to $E[g]$, we find that $E[g]$ is $O(\text{order}(\psi_{\text{inc}})\ \epsilon)$. This means that $\mathrm{Var}[g]$ scales as,

$$\mathrm{Var}[g] = \underbrace{\underbrace{E[g^2]}_{O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)} - \underbrace{(E[g])^2}_{O(\text{order}(\psi_{\text{inc}})^2\ \epsilon^2)}}_{O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)} \,. \tag{61}$$

We now have both terms in eq. (36).

Substituting eqs. (59) and (61) into eq. (36) gives the final result,

$$\mathrm{Var}[f+g] = \underbrace{\underbrace{\mathrm{Var}[f]}_{O(\text{order}(Q)^2\ \epsilon)} + \underbrace{\mathrm{Var}[g]}_{O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)}}_{O\left(\max\left\{\text{order}(Q)^2,\, \text{order}(\psi_{\text{inc}})^2\right\}\ \epsilon\right)} \,. \tag{62}$$

Thus, the path length estimator of the angle integrate intensity $\hat{\phi}$ has a variance which is the larger of $O(\text{order}(Q)^2\ \epsilon)$ and $O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)$ in the TDL.

□

Our proof demonstrates that $\mathrm{Var}[\hat{\phi}]$ is the larger of $O(\text{order}(Q)^2\ \epsilon)$ and $O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)$ in the TDL. However, it is possible to prove theorem 1 for a different estimator—such as a collision estimator or a surface crossing estimator—or a different quantity, such as the first angular moment or the second angular moment of the radiation intensity, by modifying the steps involving the derivation of the expectation. In our case, we derived the expectation for the path length estimator of the angle integrated intensity $\hat{\phi}$, and thus our proof specifically establishes that $\mathrm{Var}[\hat{\phi}]$ is the larger of $O(\text{order}(Q)^2\ \epsilon)$ and $O(\text{order}(\psi_{\text{inc}})^2\ \epsilon)$ in the TDL. If there is no inflow, then the result simplifies to $O(\text{order}(Q)^2\ \epsilon)$.

One limitation of our proof is the assumption that only a single material is present. This assumption circumvents the complications associated with the spatial variation of material properties, such as the total opacity σ_t. One example of a simplification that arises due to this assumption is that the non-constant rate exponential probability distribution function eq. (9) is replaced by the constant rate exponential probability distribution function eq. (39). Another limitation is the assumption that simulation particles can have no more than one collision.

The application that we highlight in the next section is a result that was obtained because of theorem 1.

4. Application of the Theorem

Hybrid Second Moment (HSM) is a hybrid Monte Carlo-deterministic method for solving eq. (2a) with Q defined by eq. (3) subject to the inflow boundary condition eq. (2b) without simulating scattering events [5]. Instead, the contribution of the scattering source is incorporated into the weight of the simulation particles. This necessitates an iteration to compute successive approximations of the integral in eq. (3). Instead of using the angle integrated intensity estimator to approximate the integral, the authors solve a moment system, then use the solution in place of the integral.

The Monte Carlo solve in HSM estimates the angle integrated intensity associated with the equation,

$$\mathbf{\Omega} \cdot \nabla \psi + \sigma_t \psi = \frac{\sigma_s}{4\pi} \varphi + q \,, \tag{63}$$

where $\mathbf{\Omega}, \psi, \sigma_t, \sigma_s$, and q were defined in section 2, and φ is the solution of the moment system. Equation (63) is subject to the inflow boundary condition eq. (2b). Thus, the total source function Q for eq. (63) is,

$$Q = \frac{\sigma_s}{4\pi} \varphi + q \,. \tag{64}$$

We can use theorem 1 to predict how HSM will perform in the TDL. Applying the TDL scaling eqs. (4a) to (4c) to eq. (64) shows that the terms in Q scale as,

$$Q = \underbrace{\frac{\sigma_s}{4\pi}}_{O(\epsilon^{-1})} \varphi + \underbrace{q}_{O(\epsilon)} \,. \tag{65}$$

Thus, Q for eq. (63) is $O(1/\epsilon)$, because $1/\epsilon \gg \epsilon$. By theorem 1, $\mathrm{Var}[\cdot]$ is $O(1/\epsilon)$ for estimators computed in a weighted Monte Carlo particle simulation of the transport problem defined by eq. (63) subject to the boundary condition eq. (2b), assuming that ψ_{inc} is $O(1)$ in the TDL. The authors fix the noise issue by fixing the undesirable dependence of the variance on ϵ. They do this by substituting $\psi = \bar{\varphi}/(4\pi) + \tilde{\psi}$ into eq. (63), where $\bar{\varphi}$ is an arbitrary function which they define to satisfy certain properties, including that $\varphi - \bar{\varphi}$ is $O(1/\sigma_t)$. The result is,

$$\mathbf{\Omega} \cdot \nabla \tilde{\psi} + \sigma_t \tilde{\psi} = \frac{\sigma_t}{4\pi} (\varphi - \bar{\varphi}) - \frac{1}{4\pi} (\sigma_a \varphi + \mathbf{\Omega} \cdot \nabla \bar{\varphi}) + q \,. \tag{66a}$$

They substitute $\psi = \bar{\varphi}/(4\pi) + \tilde{\psi}$ into eq. (2b), which gives a new inflow boundary condition,

$$\tilde{\psi}(\mathbf{x}, \mathbf{\Omega}) = \psi_{\mathrm{inc}}(\mathbf{x}, \mathbf{\Omega}) - \frac{1}{4\pi} \bar{\varphi}(\mathbf{x}) \,, \quad \mathbf{x} \in \partial \mathcal{D} \text{ and } \mathbf{\Omega} \cdot \mathbf{n} < 0 \,. \tag{66b}$$

We can apply theorem 1 once more, this time to the new transport problem defined by eqs. (66a) and (66b). Consider the total source function in eq. (66a). The terms scale as,

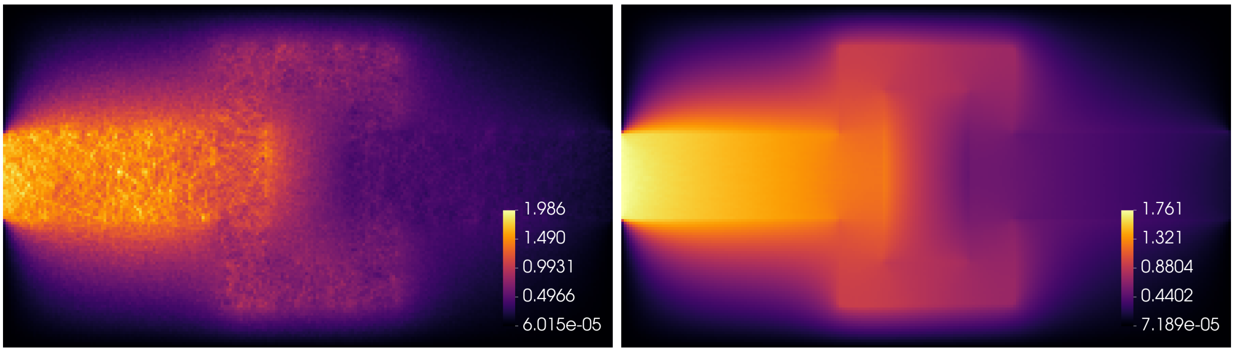
$$Q = \underbrace{\underbrace{\frac{\sigma_t}{4\pi} \underbrace{(\varphi - \bar{\varphi})}_{O(1/\sigma_t)}}_{O(1)} - \underbrace{\frac{1}{4\pi} (\underbrace{\sigma_a \varphi}_{O(\epsilon)} + \underbrace{\mathbf{\Omega} \cdot \nabla \bar{\varphi}}_{O(1)})}_{O(1)} + \underbrace{q}_{O(\epsilon)}}_{O(1)} \,. \tag{67}$$

The terms in the new inflow boundary condition eq. (66b) scale as,

$$\tilde{\psi}(\mathbf{x}, \boldsymbol{\Omega}) = \underbrace{\psi_{\text{inc}}(\mathbf{x}, \boldsymbol{\Omega})}_{O(1)} - \underbrace{\frac{1}{4\pi}\varphi(\mathbf{x})}_{O(1)}, \tag{68}$$

where we have assumed once more that ψ_{inc} is $O(1)$ in the TDL. By theorem 1, the variance of the path length estimator for the angle integrated intensity for eq. (66a) subject to the boundary condition eq. (66b) is $O(\epsilon)$.

Thus, by using theorem 1, the authors of HSM were able to take a method which has a variance that limits to infinity in the TDL, and create a method which has a variance that limits to zero in the TDL. The variance reduction procedure guided by theorem 1 allowed the HSM authors to make HSM useful, instead of useless. Figure 4 shows the result of solving a proxy problem from radiative transfer using HSM, both with and without variance reduction, with 16 million particles in each case. Variance reduction makes the noise nearly imperceptible.



(a) (b)

Figure 4: Numerical solution before (a) and after (b) applying variance reduction using theorem 1.

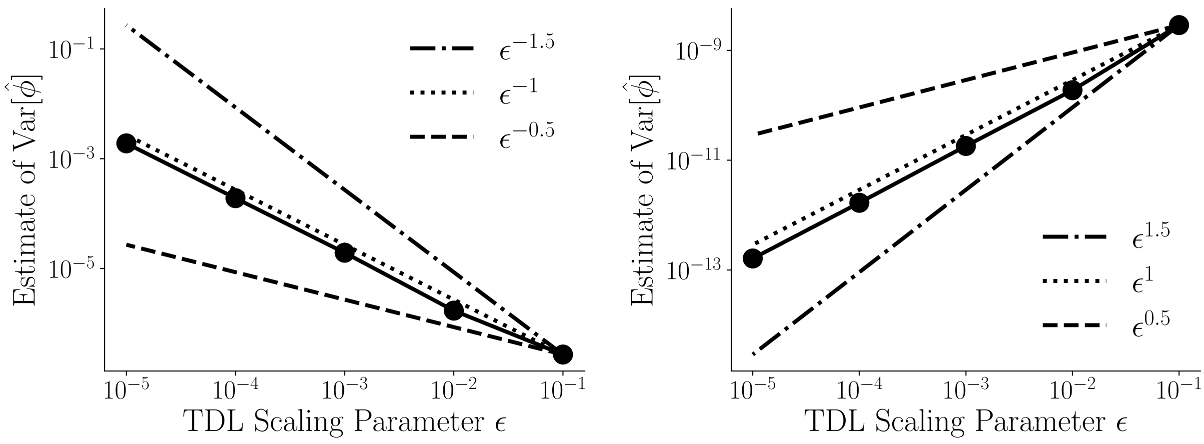
By "imperceptible", we simply mean that the pseudocolor plot in fig. 4b appears completely smooth. The pseudocolor plot in fig. 4a exhibits substantial speckling, which is a result of the noise issue: relatively long paths traversed by relatively high-weight particles create bright streaks in the plot. This high-frequency (short-wavelength) spatial variation of the numerical solution is unphysical.

The authors found that they needed approximately 500 times more particles (8 billion instead of 16 million) to achieve imperceptible noise without variance reduction. Details of the radiative transfer proxy problem problem may be found in [5].

The authors of the same publication also ran single-zone, single-material calculations in which they gradually increased the optical-thickness of the material by decreasing the TDL parameter ϵ, and estimated the variance of the angle integrated intensity. Figure 5 shows a plot of their results, reproduced with their permission. They observed the hypothesized variances, which limit to infinity and to zero as shown in fig. 5 (a) and (b), respectively. Details of the gradually-increased optical-thickness problem, which provided empirical evidence in support of the $O(1/\epsilon)$ and $O(\epsilon)$ functional form of the analytic variances, may be found in [5].

5. Conclusions

We presented a proof of a theorem describing the variance of Monte Carlo estimators in an important asymptotic regime characterized by an optically-thick, highly scattering material. Our proof is limited to the path length estimator for the angle integrated intensity in a single material for simulation particles that have no more than one collision, but we suggested ways in which one could alleviate some of these limitations. The authors of a radiative transfer method used the theorem to develop a variance reduction



(a) Variance of HSM estimator for eq. (63).

(b) Variance of HSM estimator for eq. (66a).

Figure 5: Hybrid Second Moment estimator variance before variance reduction (a) and after variance reduction (b). Reproduced with permission from the authors of [5].

technique that enabled a Monte Carlo solution estimator to achieve imperceptible noise with approximately 500 times fewer simulation particles than would be required without variance reduction.

6. Acknowledgements

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