Monte Carlo Approach to Modeling of Boundary Conditions for the Diffusion Equation

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A Monte Carlo scheme is proposed to obtain boundary conditions for the photon-diffusion equation. For a turbid medium with interfaces to nonscattering media, we introduce an interpolated boundary, at a distance of a few transport-mean-free paths from the physical boundary, which acts as the secondary source emitting photons in various directions. The ratio of the fluence rate to the flux is evaluated at both the interpolated and the physical boundaries. The derived boundary conditions are compared with other works and are supported by an independent simulation of an effective source term. [S0031-9007(98)06369-8]

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In the last decade, much attention has been focused on the applications of far-red and near-infrared diffusing-light probes to biomedical investigations such as blood oximetry and direct imaging of breast tumors. Biological tissues have some interesting optical properties in the band between about 600 and 1300 nm, which classify them as turbid media. Since their absorption coefficients (μ_a) are always negligible compared with the scattering coefficients (μ_s) [1], most propagating photons experience a large number of scattering events before they finally are absorbed or emerge from tissues through interfaces. In this case, one can easily conclude the diffusion approximation in regions not very close to a light source or boundary, which assumes that the radiance is primarily isotropic except a small directional term representing the average energy flux. With this approximation, the transport theory can be reduced to the diffusion equation [2], which has a close solution form in an infinite homogeneous turbid medium. However, in most practical situations one has to consider the boundary effects, which introduce much complexity.

Many researchers are devoted to finding an appropriate boundary condition using various methods [3–6]. An oversimplified choice is to set the fluence rate $\Phi = 0$ at the physical surface, which obviously invalidates the diffusion approximation and is totally unphysical. More sophisticated treatments include finding the ratio of fluence rate to its normal derivative at the boundary, or equivalently, a distance outside the turbid medium at which the diffusion part of the fluence rate can be extrapolated to zero. In the presence of a planar absorbing (refractive index matches between the inside and the outside of the turbid medium) interface, the solution of the Milne equation gives an extrapolation length of about $0.7l^*$ (l^* is the note of the transport-mean-free path) for isotropic scatters. When the refractive index mismatches between the turbid medium and the outer medium (e.g., the air), one has to consider the effects of internal reflection. That means the boundary is now partially absorbing. Haskell *et al.* [3] have evaluated the ratio of the fluence rate to the flux at the physical surface, following the partial-current treatment of Keijzer *et al.* [6]. They argued that Fresnel reflection would relieve violation of the diffusion approximation thus warranting the expression of the radiance in terms of the fluence rate and the flux at the physical surface. Their results rely importantly on the effective reflection coefficient R_{eff}, which was evaluated on the assumption that the radiance incident on the surface satisfies $P1$ approximation. However, this could not be the case in many realistic conditions. Freund [4] also included an effective reflection coefficient in both the transport theory and the Milne theory, then obtained two sets of approximate boundary conditions for 1D, 2D, and 3D. He took the results from Milne theory as preferable because it involves the photon density directly. For 3D models, the extrapolation lengths provided by the Milne theory are very close to those given in the literature [3]. Nonetheless, Jiang *et al.* [7] recently claimed that the ratio determined experimentally is much smaller. Unfortunately, they did not give details of how their data were obtained and even did not provide the value.

The Monte Carlo method stands alone when analytic approaches have difficulties in giving a satisfactory solution of a problem. It has been frequently used to solve transport problems. Ordinary Monte Carlo models trace a huge number of photon trajectories from the source to the detector. Then a variety of optical properties characterizing the light-propagation process can be estimated [8]. To extract an appropriate boundary condition, one needs to have a close look at the statistic behavior of photons near the interface. So we developed a specified simulation scheme accounting for this end.

As shown in Fig. 1, a semi-infinite turbid medium model is considered with a planar interface to a nonscattering medium, say, the air, and with light sources located deep inside the turbid medium. To take advantage of the diffusion approximation, we introduce an interpolated boundary, a plane a few l^*'s away from the physical boundary. It is in the thin slab restricted by both the

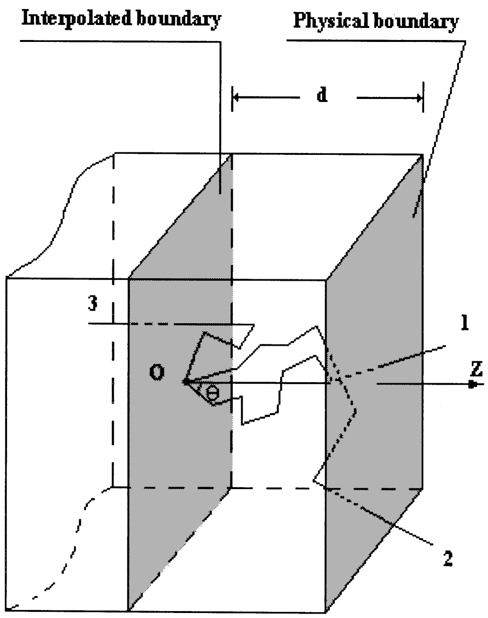

FIG. 1. Geometry of a semi-infinite turbid medium with a planar interface to the air. Two shaded planes, the physical boundary (right) and the interpolated boundary (left), restrict a thin slab in which photon trajectories are traced. In our simulation, all photons entering the slab are emitted by a secondary point source located at the origin, as illustrated by the three sample trajectories labeled 1, 2, and 3.

interpolated and the physical surfaces that photon trajectories are traced. Each area element on the interpolated surface acts as a secondary source that emits photons into the slab. Then these photons are traced until they eventually leave the slab through either the interpolated or the physical boundary. Since the thickness of the slab is rather small, there are generally limited scattering events occurring for a single trajectory. So we can implement our simulation totally according to the physical picture without much simplification while keeping the computation time acceptable.

The origin of the coordinate system is located at the interpolated surface while the normal pointing outward coincides with the polar axis. We use the polar angle θ and azimuthal angle φ characterizing the flight direction of a photon. For simplicity, the secondary source of an area element around the origin can be replaced by a point source at, say, the origin without any disadvantage. When a photon is launched into the slab, its initial direction is randomly generated with a probability density determined by the angular distribution of the radiance, which is unknown at this moment. Nevertheless, the diffusion approximation makes the situation better by writing down the radiance $L(\vec{s})$ in terms of only the fluence rate Φ and the flux $\vec{J}$,

$$L(\vec{s}) = \frac{1}{4\pi}\Phi + \frac{3}{4\pi}\vec{J}\cdot\vec{s}\,, \tag{1}$$

where $\vec{s}$ is a unit vector, and Φ and $\vec{J}$ are defined as the following:

$$\Phi = \iint_{4\pi} L(\vec{s})\,d\Omega\,, \tag{2a}$$

$$\vec{J} = \iint_{4\pi} L(\vec{s})\vec{s}\,d\Omega\,. \tag{2b}$$

Without loss of generality, our model possesses transport symmetry along any direction in the interpolated plane, so we can rewrite Eq. (1) as

$$L(\theta) = \frac{1}{4\pi}\Phi + \frac{3}{4\pi}J_z\cos\theta\,. \tag{3}$$

Because the ratio of J_z to Φ needs to be evaluated in the process of simulation, we do not know the probability density related to $L(\theta)$ in advance. The following procedure is adopted to overcome this difficulty. At first, a certain number of photons fly into the slab in random directions with a probability density $W(\theta)$ in accord with uniform radiance. The photons finally returning back contribute to $L(\theta)$ with $\pi/2 < \theta < \pi$; thus both J_z and Φ obtain rough values at this time. These values, of course, will not satisfy Eq. (3). Next, we need to launch additional photons gradually with the $W(\theta)$ modified by a multiplication factor $\cos\theta$, which comes from the flux term, until Eq. (3) achieves self-consistency. Then the ratio of the fluence rate to the flux at the interpolated boundary R_{int} is eventually obtained together with R_{phy}, the corresponding value at the physical boundary.

Modeling of the scattering process has been discussed in the literature [9]. The path length l between two subsequent scattering events is sampled according to Beer's law, in terms of the scattering mean-free path length l_s. It is well accepted that a single scattering event possesses cylindrical symmetry with respect to the incident direction, while the polar angle of scattering θ_s is determined by the light-scattering phase function $f(\theta_s)$. For biological tissues, the Henyey-Greenstein (H-G) phase function is regarded as a good approximation of an actual phase function measured experimentally, so it is adopted in our simulations. The only parameter for this kind of phase function is an asymmetry factor g, which is a characteristic anisotropy of scattering in θ_s. In the case of nonabsorbing media, the transport-mean-free path can be defined as

$$l^* = \frac{l_s}{(1-g)}\,. \tag{4}$$

We have made simulations for models with scattering parameters in the range typically found in biological tissues. Table I provides results for media with no absorption ($\mu_a = 0$) and with the refractive index $n = 1.33$. Various anisotropy factor g and thickness of the slab d in the scale of l^* have been used to yield the ratio $\Phi/3|\vec{J}|$ at both the interpolated and the physical surfaces. Bearing in mind that the flux is given by Fick's law $\vec{J} = -l^*\nabla\Phi/3$ and remains unchanged along the z axis, one can easily figure out that the ratio $\Phi/3|\vec{J}|$ will decrease by 1 with d/l^* increasing by a unit in the area where the diffusion

TABLE I. The ratio of the fluence rate to the flux and corresponding extrapolation length for media with $n = 1.33$, $\mu_a = 0$.

		$\Phi/3\lvert\vec{J}\rvert$		
d/l^*	g	Interpolated boundary	Physical boundary	Δ/l^*
	0.7	2.12 ± 0.01	2.12 ± 0.01	1.12 ± 0.01
1	0.8	2.06 ± 0.01	2.54 ± 0.01	1.06 ± 0.01
	0.9	2.00 ± 0.01	3.60 ± 0.01	1.00 ± 0.01
	0.7	3.12 ± 0.02	2.12 ± 0.04	1.12 ± 0.02
2	0.8	3.06 ± 0.02	2.49 ± 0.05	1.06 ± 0.02
	0.9	3.00 ± 0.02	3.62 ± 0.07	1.00 ± 0.02
	0.7	4.13 ± 0.02	2.19 ± 0.04	1.13 ± 0.02
3	0.8	4.07 ± 0.02	2.51 ± 0.05	1.07 ± 0.02
	0.9	4.03 ± 0.02	3.67 ± 0.07	1.03 ± 0.02
	0.7	5.16 ± 0.03	2.15 ± 0.04	1.16 ± 0.03
4	0.8	5.13 ± 0.03	2.51 ± 0.05	1.13 ± 0.03
	0.9	5.03 ± 0.03	3.61 ± 0.07	1.03 ± 0.03

theory is valid. The values for ratios at various interpolated boundaries demonstrate that the diffusion theory keeps valid up to one l^* inside the physical surface, as shown in the third column of Table I. These values lead to an extrapolation length which can act as an appropriate boundary condition for solving the diffusion equation inside the turbid medium correctly. For example, a medium with $g = 0.9$ and refractive index $n = 1.33$ has an extrapolation length $1.0l^*$, obviously smaller than $1.7l^*$ given in the literature [3]. In fact, the extrapolated length will increase gradually when the anisotropy factor gets smaller and will be rather close to $1.5l^*$ with isotropic scatters. This has never been indicated in former works. For biomedical tissues, the typical value of g is found between 0.7 and 0.95. So the correction we give is remarkable. The values for ratios listed in the fourth column show strong violation of the diffusion approximation. If we extrapolate these values to zero, we will obtain much larger extrapolation lengths, as predicted by Freund [3]. Therefore, they are useless in this case. We also tested many kinds of phase functions other than the H-G phase function, but found trivial differences. Simulations for various refractive indexes indicate that the increasing surface reflection will yield a larger extrapolation length, as one can expect intuitively. In the presence of a totally absorbing interface, our model gives an extrapolation length $0.7l^*$, almost independent of g.

Next, we provide an example to show the importance of our findings. Let us still consider a semi-infinite turbid medium. Now a light source is placed outside and is collimated to irradiate the surface perpendicularly. Evaluation of the signals collected by a detector depends a lot on the modeling of the light source. It is well accepted that any detector at a large separation from the source would see an isotropic point source located one l^* into the medium. To include the boundary effect, one can resort to the method of image. The original source can be replaced by an effective one with the dipole moment determined by the boundary condition as in the following:

$$\text{dipole moment} = (\text{light source strength}) \times (2l^* + 2\Delta)\,, \tag{5}$$

where Δ is the extrapolation length. Since our model gives a much smaller Δ, the predicted dipole moments get smaller correspondingly. To validate our data, another simulation has been conducted to estimate the effective source term. We traced photons from the entrance point to reach a given transport path length and obtained corresponding spatial distribution. Then the center of mass (average penetration depth of photon) was evaluated. Since a portion of photons would have escaped through the boundary, the longer the path we allow photons to transport, the fewer photons remained, and the deeper the center of mass located into the turbid medium. However, a consistent dipole moment should be achieved, independent of the transport path length provided that they are sufficiently large. This can be done only with appropriate boundary conditions. Table II shows the results for a model medium with refractive index 1.33 and $g = 0.8$. The dipole moments related to our extrapolation length ($\Delta/l^* = 1.06$) are almost identical in contrast to the constantly decreasing values derived with the boundary condition ($\Delta/l^* = 1.7$). Furthermore, they are rather close to that predicted by Eq. (5).

In conclusion, our model provides a numerical method to find boundary conditions for the diffusion equation. At the physical boundary, the fluence rate always dominates the flux when internal reflection exists. This fact,

TABLE II. Values of the dipole moments (DM) for various transport lengths (TL) in a model medium with $g = 0.8$, $n = 1.33$. The strength of incident light is set to unit. RS is the relative strength which represents the portion of photons remaining in the turbid medium, while APD stands for the average penetration depth.

TL/l^*	50	75	100	125
RS	0.523 ± 0.001	0.477 ± 0.001	0.421 ± 0.001	0.381 ± 0.001
APD/l^*	2.540 ± 0.004	3.206 ± 0.004	3.768 ± 0.004	4.288 ± 0.004
DM: $\Delta/l^* = 1.06$	4.05 ± 0.01	4.07 ± 0.01	4.07 ± 0.01	4.08 ± 0.01
$\Delta/l^* = 1.7$	4.77 ± 0.01	4.68 ± 0.01	4.61 ± 0.01	4.56 ± 0.01

however, does not necessarily mean that the diffusion approximation also survives there. Generally, the ratio at the physical surface and the related extrapolation length is too large to be appropriate. On the other hand, the ratio at an interpolated boundary leads to correct extrapolation lengths for biomedical tissues. Also, our model makes it easy to estimate the angular distribution of the radiance emerged from a turbid medium.

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