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Hybrid model of light propagation in random media based on the time-dependent radiative transfer and diffusion equations

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ABSTRACT

Numerical modeling of light propagation in random media has been an important issue for biomedical imaging, including diffuse optical tomography (DOT). For high resolution DOT, accurate and fast computation of light propagation in biological tissue is desirable. This paper proposes a space–time hybrid model for numerical modeling based on the radiative transfer and diffusion equations (RTE and DE, respectively) in random media under refractive-index mismatching. In the proposed model, the RTE and DE regions are separated into space and time by using a crossover length and the time from the ballistic regime to the diffusive regime, $\rho_{DA} \sim 10/\mu_t'$ and $t_{DA} \sim 20/\nu\mu_t'$ where μ_t' and ν represent a reduced transport coefficient and light velocity, respectively. The present model succeeds in describing light propagation accurately and reduces computational load by a quarter compared with full computation of the RTE.

1. Introduction

Diffuse optical tomography (DOT) offers the potential to monitor oxygenation in biological tissue noninvasively [1,2]. It requires an algorithm to estimate the distribution of optical properties in tissue from measurements at the boundaries of the medium studied [3]. The algorithm essentially consists of two parts. One is a forward model to calculate the light propagation in a medium and the resultant outward reemissions at the boundary of the medium. The other is an inverse model to search for a distribution of the optical properties by minimizing differences between the calculated and the experimental data.

As a forward model, it has been widely accepted that the radiative transfer equation (RTE) provides an accurate description of light propagation phenomena by comparing with experimental data using tissue phantoms [4]. Due to this, the applicability of the RTE has been investigated to improve DOT images [5]. With its accurate calculations of light properties, the RTE still suffers from the disadvantage of high computation load due to the complexity of the integro-differential equations and a high number of independent variables. Thus, the most forward models are based on the diffusion equation (DE) [6,7], which is deduced from the RTE. The use of the DE reduces computational times and memory requirements significantly compared to that of the RTE. However, the DE is known to be invalid in the vicinity of sources and absorbing objects [8]. As a result DE-based models are susceptible to errors around these sources and objects, leading to low quality DOT images.

Alternative models for the accurate and efficient calculation of light propagation have also been proposed [9–14], and among these a hybrid model based on the RTE and the DE is one of the most promising approaches. Tarvanien et al. have

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proposed the hybrid model in frequency domain [10–12], and Gorpas et al. have applied this model to fluorescence imaging [13,14]. It has been successfully shown that the light propagation calculated from this model is in good agreement with the RTE calculations. The hybrid model is based on the DE giving accurate results far from sources. In the model, the whole region of a medium is divided into the RTE region at short source–detector distances ($\rho < \rho_{DA}$) and the DE region at long distances ($\rho > \rho_{DA}$), where ρ_{DA} represents a crossover length from the ballistic regime to the diffusive regime [15]. Despite the good results, the estimates of ρ_{DA} involve trial and error, and are medium-dependent. As a result there is still a need for a model where ρ_{DA} is expressed in terms of the optical properties, independent of the media involved. Also, due to high computational loads of solving the time-dependent RTE, only a few publications showing the results of the RTE in time-domain are found [16].

This paper extends the concept of the hybrid model in the steady state legitimately to the time domain as the time domain has more information of light propagation than a steady state system. In this extended hybrid model, the RTE and DE regions are divided into space and time by using the crossover length ρ_{DA} and a crossover time $t_{DA} \sim \rho_{DA}/\mathrm{v}$. To estimate the ρ_{DA} and t_{DA} without reference to media, the time development of light propagation based on the RTE and the DE are investigated with the refractive-index mismatched boundary condition. The accuracy and computational efficiency of the proposed model is tested by a comparison with numerical results based on the RTE.

This paper is organized as follows. The following section provides a brief explanation of numerical models of the RTE, DE, and the hybrid model proposed here. Section 3 provides numerical results of the light propagation based on the three models under several conditions. Finally, conclusions are detailed in Section 4.

2. Numerical model

This paper uses homogeneous 2D rectangular media (3.2 cm $\times$ 4.0 cm) as shown in Fig. 1 throughout.

2.1. Radiative transfer equation

Light propagation in random media is described by the intensity $I(\mathbf{r}, \mathbf{\Omega}, t)$, which is the energy distribution of photons described by the position $\mathbf{r} = (x, y)$, angular direction $\mathbf{\Omega} = (\Omega_x, \Omega_y)$, and time t. Considering photon–matter interactions as transit, absorption, and scattering, this makes it possible to derive the RTE [17]

$$\left[\frac{\partial}{v\partial t} + \mathbf{\Omega}\cdot\nabla + \mu_t(\mathbf{r})\right] I(\mathbf{r}, \mathbf{\Omega}, t) = \mu_s(\mathbf{r}) \int_S d\mathbf{\Omega}' P(\mathbf{\Omega}, \mathbf{\Omega}') I(\mathbf{r}, \mathbf{\Omega}', t) + q(\mathbf{r}, \mathbf{\Omega}, t), \tag{1}$$

where $\mu_t(\mathbf{r})$ is given by the sum of the absorption $\mu_a(\mathbf{r})$ and scattering coefficients $\mu_s(\mathbf{r})$, v is the velocity of light in the target medium, $P(\mathbf{\Omega}, \mathbf{\Omega}')$ is a scattering phase function providing a scattering probability from the $\mathbf{\Omega}'$ before scattering to the $\mathbf{\Omega}$ after scattering, and $q(\mathbf{r}, \mathbf{\Omega}, t)$ is the light source. In the above formulation, polarization and inelastic scattering of photons are disregarded.

Like other studies the present study employs the Henyey–Greenstein phase function for $P(\mathbf{\Omega}, \mathbf{\Omega}')$ due to its simplicity [18] and for the two-dimensional cases, this function is given as

$$P(\mathbf{\Omega}\cdot\mathbf{\Omega}') = \frac{1}{2\pi}\frac{1-g^2}{1+g^2-2g\mathbf{\Omega}\cdot\mathbf{\Omega}'}, \tag{2}$$

where the anisotropic parameter g is defined as an expectation value of $\mathbf{\Omega}\cdot\mathbf{\Omega}'$ for the function $P(\mathbf{\Omega}, \mathbf{\Omega}')$. In this paper, the value of g is chosen to be zero or positive for modeling isotropic and forward scatterings in biological tissue and phantoms. Due to the elastic scattering, P satisfies the normalized condition $\int d\mathbf{\Omega} P(\mathbf{\Omega}\cdot\mathbf{\Omega}') = 1$.

The source $q(\mathbf{r}, \mathbf{\Omega}, t)$ takes the form of a delta function as $\delta(\mathbf{r}-\mathbf{r}_s)\delta(\mathbf{\Omega}-\mathbf{\Omega}_s)\delta(t)$, where $\mathbf{r}_s$ and $\mathbf{\Omega}_s$ denote the position and the angular direction of an incident pulse, respectively.

At the boundary, the refractive-index mismatching is considered, this is a more realistic boundary condition than the non-reentry boundary condition. The reflection and refraction at the boundary are described by Fresnel's law, which gives the reflectivity $R(n, \theta)$ as

$$R(n,\theta) = \begin{cases} \dfrac{1}{2}\left[\dfrac{\sin^2(\theta_r-\theta)}{\sin^2(\theta_r+\theta)} + \dfrac{\tan^2(\theta_r-\theta)}{\tan^2(\theta_r+\theta)}\right], & \theta < \theta_c \\ 1, & \theta \geq \theta_c \end{cases} \tag{3}$$

where n is the relative refractive index of the medium, θ is an angle between the outgoing normal vector $\mathbf{e}_n$ and $\mathbf{\Omega}$ as shown in Fig. 1(a), the refraction angle $\theta_r = \sin^{-1}(n \sin\theta)$ is obtained by Snell's law, and θ_c represents the critical angle. The transmissivity $T(n, \theta)$ is given by $1 - R(n, \theta)$.

To obtain numerical solutions of the RTE, this equation is replaced by a set of linear equations by using the upwind-discrete ordinate and finite-difference scheme [4]. In this scheme, $I(\mathbf{r}, \mathbf{\Omega}, t)$ is discretized as $I_{i,j,k,m}$, where i, j, k, and m denote the indices of the discrete spatial (x_i, y_j), angular $\mathbf{\Omega}_k$, and temporal t_m variables. The integration term in the equation is calculated based on the extended trapezoidal rule, $\int d\mathbf{\Omega}\, PI \sim \sum_k w_k P_{kk'} I_k$ with a weight factor w_k and angular index k. Commonly, w_k is given by $2\pi/N_\theta$ with the number of discrete angles N_θ. However, when N_θ is not sufficiently large, normalization of P is not possible, i.e. when $\sum_k w_k P_{kk'} \neq 1$ especially at large values of g. For numerical calculations to converge, a modified weight factor is adopted, $w_k^{(mod)} = w_k(\sum_l w_l P_{lk})^{-1}$ [19] in this study. The temporal derivative is approximated by the forward Euler scheme [16].

2.2. Diffusion approximation

In the diffusion approximation (DA), a first order approximation of $I(\mathbf{r}, \mathbf{\Omega}, t)$ with respect to $\mathbf{\Omega}$ and Fick's law is assumed. Then, the diffusion equation (DE) can be derived from the RTE

$$\left[\frac{\partial}{v\partial t} - D\nabla^2 + \mu_a\right]\Phi(\mathbf{r}, t) = q_{DE}(\mathbf{r}, t), \tag{4}$$

where the fluence rate $\Phi(\mathbf{r}, t)$ is given by $\int d\Omega\, I(\mathbf{r}, \mathbf{\Omega}, t)$, the diffusion coefficient D is given by $[2(1-g)\mu_s]^{-1}$ for the time domain system [20,21], and the isotropic source $q_{DE}(\mathbf{r}, t)$ is given by $\int d\Omega\, q(\mathbf{r}, \mathbf{\Omega}, t)$. The refractive-index mismatched boundary condition is reduced to the Robin