The Propagation of Laser Light in Skin by Monte Carlo-Diffusion Method: A Fast and Accurate Method to Simulate Photon Migration in Biological Tissues

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Abstract:

Introduction: Due to the importance of laser light penetration and propagation in biological tissues, many researchers have proposed several numerical methods such as Monte Carlo, finite element and green function methods. Among them, the Monte Carlo method is an accurate method which can be applied for different tissues. However, because of its statistical nature, Monte Carlo simulation requires a large number of photon pockets to be traced, so it is computationally expensive and time-consuming. Although other numerical methods based on the diffusion method are fast, they have two important limitations: first, they are not valid near the bounder of sample and source, and second, their accuracy is less than Monte Carlo method.
Method: In this study, we combine the accuracy of Monte Carlo method and speed of the diffusion method. This hybrid method is faster than Monte Carlo Method and its accuracy is higher than the diffusion method.
Results: We first evaluate this hybrid model and the reflectance of a biological phantom is calculated by Monte Carlo method and this hybrid model. Then the propagation of laser light in the skin tissue has been studied.
Conclusion: In this study, a combined method based on the Monte Carlo method and the diffuse equation is introduced. This hybrid method is five times faster than Monte Carlo Method, and its accuracy is higher than the diffusion method. The propagation of laser light in skin has also been studied by this hybrid method and its accuracy shows that it can be applied for laser penetration in biological tissues. It seems that this method is good for photo dynamic therapy (PDT) and optical imaging.
Keyword: biological tissue; method, monte carlo; diffusion method; photon migration

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Introduction

Biomedical optics or light-tissue interaction is a rapidly growing subject of science. That is because, light sources such as coherent light like lasers and other non-coherent sources like Xenon lamp have made much progress in medicine, especially in dermatology and ophthalmology (1). In the laser- tissue interaction, it is very important to know how the laser light is propagated inside

a biological tissue during laser irradiation (2-3). The light distribution in a biological tissue depends on optical properties of tissue (4-6), and also one can inversely deduce the optical properties from measurable quantities (7-9). One of these quantities is the diffuse reflectance. Therefore, we need an accurate model to relate the diffuse reflectance and optical properties of a tissue (9).

One way to understand the light distribution inside the tissue is to solve the radiation transfer equation (1,10). Since it is very difficult to solve it in complex geometries, the Monte Carlo simulation can be applied. Monte Carlo simulation is very flexible inside complex geometries, and its accuracy has also been tested experimentally (11-13). But, because of its statistical nature, we have to trace large numbers of photon's path too in order to get rational results. So it is time-consuming (14).

Another way to solve the radiation transport equation is to approximate it with diffusion equation (1, 15-16). We can use diffusion theories to approximate physical quantities of light transport in tissue, but they are not valid near the source, or near the boundary where the photon intensity is strongly anisotropic (1-2, 17).

In this paper, first, we used the hybrid model of Monte Carlo simulation and diffusion theory to compute the diffuse reflectance of pencil narrow photon beam incident upon a semi infinite homogeneous medium with given optical properties. This method combines the speed advantage of diffusion theory and accuracy of Monte Carlo simulation. Then, we applied this method to the multi layered skin tissue and computed the diffuse reflectance, where ρ is the distance between the observation and the incident points of the laser beam on the medium surface.

$$R_d(\rho)$$

Review of Theory

At first, we explain the Monte Carlo method to simulate photon migration in biological tissues. The origin of the coordinate system is the point of photon incidence on the tissue surface, and the z axis points downward into the tissue. The radial coordinate and the polar angle are denoted by ρ and θ, respectively.

The Monte Carlo simulation step is based on references number 2, 13 and18. Implicit photon capture is used to improve the efficiency of the

Monte Carlo simulation. Each photon packet is initially assigned a weight 1 and is injected orthogonally into the tissue at the origin. If there is a mismatched boundary at the tissue surface, then some specular reflectance will occur according to Fresnel reflection. Then a step size is chosen statistically by using (19):

$$S = \frac{-\ln(\xi)}{\mu_a + \mu_s}$$ [1]

Where ξ is a random number distributed uniformly between 0 and 1. μ_a and μ_s are absorption and scattering coefficients, respectively. In most biological tissues, the majority of scattered light guides in forward direction. So, the biological tissue has anisotropy, and it is convenient to define a phase function $p(\theta)$ of a photon to be scattered by an angle θ . If $p(\theta)$ is a constant and not dependent on θ, the media is called isotropic, otherwise, it is anisotropic media. Experiments show the mean value of phase function g is a number between -1 and +1. Where g = 1 denotes purely forwarded scattering, and g = -1 purely backward scattering, and g = 0 isotropic scattering. Most biological tissues have g > 0.7 (20).

Once the photon has taken a step, some attenuation of the photon weight due to the absorption by the interaction site must be calculated. The amount of weight loss is the photon weight at the beginning of the step multiplied by(21).

$$\frac{\mu_a}{\mu_a + \mu_s}$$

Now, the photon is ready to be scattered. A new photon direction is statistically determined by the Henyey-Greenstein phase function according to the anisotropy factor g (10). Then a new step size is generated, and the process is repeated until the photon weight falls below a threshold value.

As mentioned earlier, the diffusion theory is not valid near the boundary. So, we can use similarity relations and convert the photon packet into deep isotropic photon sources in the tissue. The similarity relations allow conversion from the anisotropic scatterers into isotropic scatterers with a reduced scattering coefficient μ'_s equal to, while the absorption coefficient is kept the same (22,17).

$$\mu_s(1-g)$$

We can use Monte Carlo simulation for this conversion, and we know that the diffusion theory is accurate for deep photons. A critical depth Z_c is defined and is chosen to be one mean free path, (mfp). Below Z_c, both diffusion theory and

similarity relations can be applied. The z = Z$_c$ plane is called the critical plane [2].

During the Monte Carlo simulation, if the photon packet crosses the surface boundary into the ambient medium, the photon weight contributes to the Monte Carlo reflectance R$_{mc}$(ρ). If the photon packet crosses the critical plane, we should statistically determine a new direction for photon. If the z-directional cosine is positive, we should move the photon packet a fixed step of 1mfp' which is the mean free path for the converted isotropic scattering medium. At the end of this step, the photon will lose weight due to the absorption by the interaction site. The remaining weight of the photon will be recorded into the source function S (ρ, z).

As discussed in reference number 23, the fluence due to a point source at depth in a semi-infinite medium can be forced to zero on a plane by introducing a negative image source of photons above the plane as illustrated in Figure 1.

The fluence for the single source in a semi-infinite medium is given as the sum of the fluence for the source and the image source calculated in an infinite medium. For a photon source at a depth Z_0, the distance from the extrapolated boundary is $Z_0 + Z_b$, and the image source will be at a height $Z_0 + Z_b$ above the extrapolated boundary, where $Z_b = 2AD$. A is related to the internal reflection r_d. The value of A is determined by [2]:
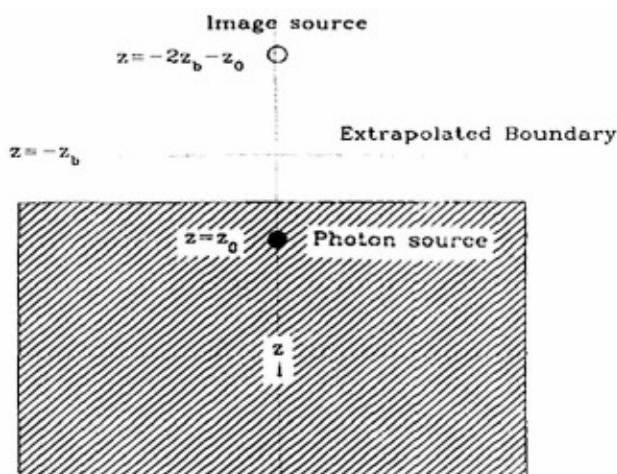
[2]

$$A = \frac{1 + r_d}{1 - r_d}$$

Figure 1. The position of the negative image source and the extrapolated boundary.

$$r_d = -1.440\left(\frac{n_m}{n_v}\right)^{-2} + 0.710\left(\frac{n_m}{n_v}\right)^{-1} + 0.668 + 0.0636\left(\frac{n_m}{n_v}\right) \quad [3]$$

Where n_m and n_v are refraction index of tissue and the ambient medium, respectively. And D is the diffusion constant.

[4]

$$D = \frac{1}{3(\mu_a + \mu'_s)}$$

The green's function for diffuse reflectance at (ρ,θ,z=0) forms a point source at (ρ', θ',z') is given by[2]:

$$R(\vec{r} - \vec{r}') = \frac{1}{4\pi}\left[z'(\mu_{eff} + \frac{1}{r_1})\frac{\exp(-\mu_{eff}r_1)}{r_1^2} + (z'+2z_b)(\mu_{eff} + \frac{1}{r_2})\frac{\exp(-\mu_{eff}r_2)}{r_2^2}\right] \quad [5]$$

Where r_1, r_2 and μ_{eff} are:

$$r_1 = [(z - z')^2 + \rho^2 + \rho'^2 - 2\rho\rho'\cos(\theta - \theta')]$$

$$r_2 = [(z + z' + 2z_b)^2 + \rho^2 + \rho'^2 - 2\rho\rho'\cos(\theta - \theta')]$$

$$\mu_{eff} = \{3\mu_a[\mu_a + \mu'_a]\}^{1/2}$$

Because of the cylindrical symmetry of the problem, we can choose the observation point at $\theta = 0$.

When Monte Carlo step of hybrid simulation is finished, the source function gives the total photon weight in a grid element. The diffuse reflectance resulting from a distributed source is calculated by:

$$\left[R_{diff}(\rho) = \int_0^\infty \int_0^\infty \int_0^{2\pi} \frac{S(\rho', z')}{\Delta VN} R(\vec{r} - \vec{r}')\rho' d\rho' d\theta' dz' = \sum_{i=0}^{N_z - 2}\sum_{j=0}^{N_\rho - 2} \frac{S(\rho_i, Z_j)}{(\pi N)} \int_0^\pi R(\vec{r} - \vec{r}')d\right]\theta'$$

[6]

N is the number of photons. The integration over θ' in Eq. [6] was done with Gaussian quadrature. The final diffuse reflectance will be the sum of the reflectances computed by the initial Monte Carlo step and the subsequent diffusion-theory step:

[7]

$$R_d(\rho) = R_{mc}(\rho) + R_{diff}(\rho)$$

Result

First, we solve the problem for a semi-infinite medium with a matched refractive index and with the optical parameter of $\mu_a = 0.1\,cm^{-1}$ and $\mu'_s = 10\,cm^{-1}$.

A grid system is set up on the cylindrical coordinate system in the ρ and z directions. The number of grid elements in the ρ and z direction is 200; and the grid separations along the ρ and the z coordinates are 5×10^{-3} cm. The size of the grid system seems to be sufficiently large, because

the source terms tend to zero around the edge of the grid system, as we have shown in Figure 2 and Figure 3.

We have used 100000 photon packets both in pure Monte Carlo simulation and the hybrid model. The result of final diffuse reflectance obtained from both models is shown in Figure 4.

Figure 4 shows that there is an agreement between both models, whereas the hybrid model runs 5 times faster than the pure Monte Carlo simulation.

We have also shown the $R_{mc}(\rho)$ which is scored during the Monte Carlo step of the hybrid model. The comparison between $R_{mc}(\rho)$ and $R_d(\rho)$ illustrates the contributions of each step of the hybrid model.

We have also plotted the difference between the average values of the hybrid model and of the pure Monte Carlo model divided by the average values

of the pure Monte Carlo simulation in Figure 5.

As we mentioned earlier, the diffusion-theory is accurate when the absorption coefficient is much less than the reduced scattering coefficient of the medium. Therefore, the hybrid model will have this limitation too.

We have also applied the hybrid model to the multi layered skin and compared it with pure Monte Carlo simulation in Figure 6.

The optical properties of skin layers are shown in Table 1.

The number of grid elements in z and ρ directions is 200, and the grid separations along the ρ coordinate is 0.001cm and along the z coordinate is $5 \times 10_{-3}$ cm. We have used 1000000 number of photon packets for both models. The run time of hybrid model is two times faster than the pure
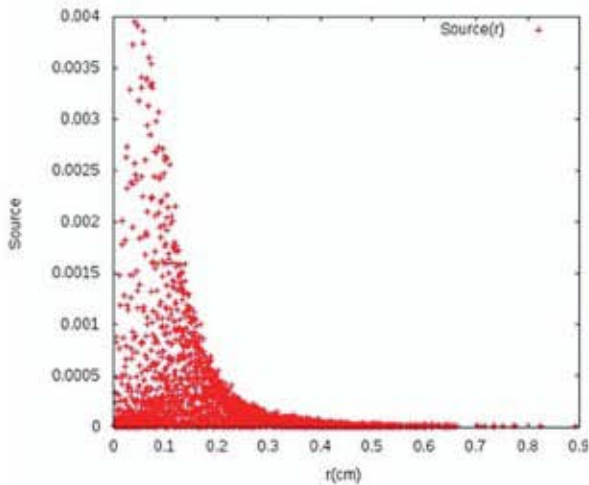

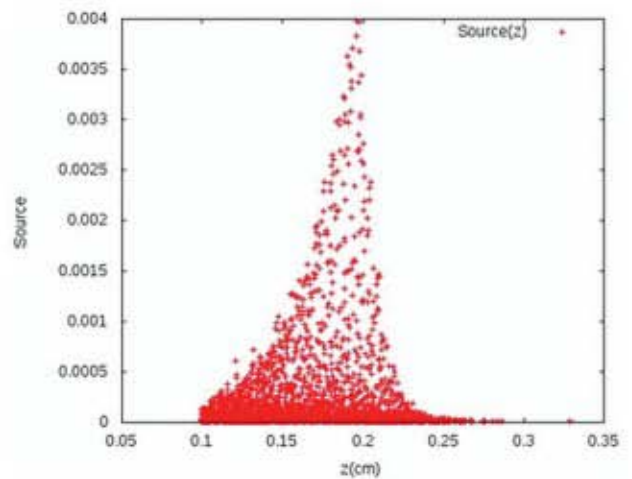Figure 2. Source intensity versus radius
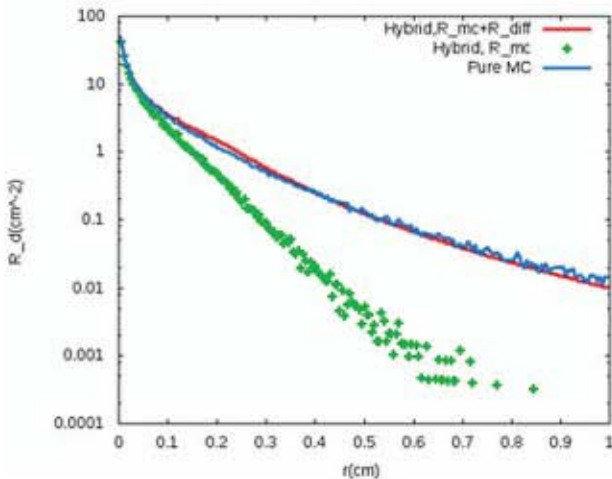

Figure 3. Source intensity versus Z

Figure 4. Diffuse reflectance for a medium with matched refractive index
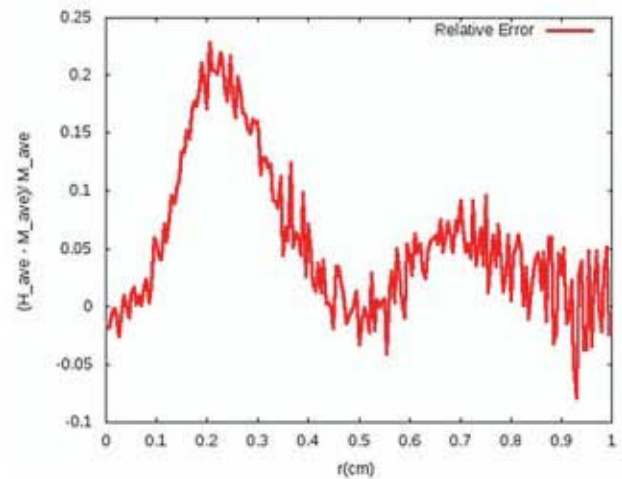

Figure 5. Difference between the average values of the hybrid model and of the pure Monte Carlo model divided by the average values of the pure Monte Carlo simulation.
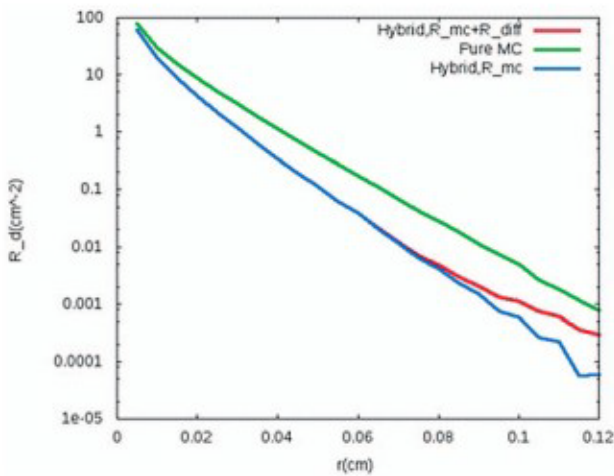
Figure 6. Diffuse reflectance of skin for Zc =0.012 cm

Table 1. The optical properties of skin layers used in hybrid model.

Skin Layer	μa(cm-1)	μs(cm-1)	g	n	Depth (μm)
Epidermis	32	165	0.72	1.4	100
Dermis	23	227	0.72	1.4	200
Dermis with plexus superficialis	40	246	0.72	1.4	200
Dermis	23	227	0.72	1.4	900
Dermis with plexus profundus	46	253	0.72	1.4	600

Monte Carlo simulation. The critical plane is chosen to be 0.012 cm. If we increase the critical plane depth to 0.02 cm, we can see that the result of hybrid model fits better with the result of pure Monte Carlo simulation. We have compared the hybrid model and pure Monte Carlo simulation for Zc=0.02 in Figure 7.
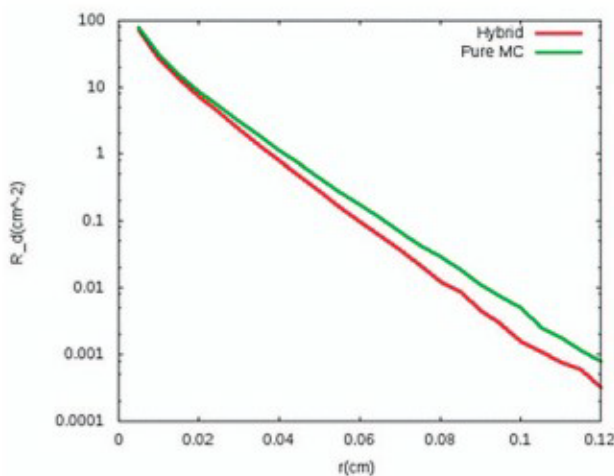

Figure 7. Diffuse reflectance of skin for Zc =0.02 cm

Conclusion

The Monte Carlo method is an accurate method to simulate photon migration in biological tissues. However, because of its statistical nature, Monte Carlo simulation requires a large number of photon pockets to be traced, so it is computationally expensive and time-consuming. Although other numerical methods based on the diffusion method are fast, they have two important limitations including low precision near to boundary of sample; and its accuracy is lower than Monte Carlo method. In this study, we combined the accuracy of Monte Carlo method and speed of the diffusion method. This hybrid method is five times faster than Monte Carlo Method, and its accuracy is higher than the diffusion method. The propagation of laser light in skin has also been studied by this hybrid method and its accuracy shows that it can be applied for laser penetration in biological tissues. It seems that this method is good for PDT and optical imaging.

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