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Computational analysis and Monte Carlo simulation of wave propagation

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Abstract: Computational analysis and modelling of wave propagation and interaction with objects are essential to help understand the fundamental problems of wave travelling. Though various methods have been proposed to model the wave propagation procedures, Monte Carlo simulation plays important role as an effective method to trace individual phone history, based on the statistics of large photon population sample to approach the wave propagation in scattering tissue objects. This paper represent our computational modelling and investigation of the Monte Carlo simulation of light propagation in scattering objects. Computer algorithms were developed to simulate the photo migration using different attenuation coefficients in the model. Results show that our Monte Carlo simulation of light propagation is capable to simulate the three-dimensional light-tissue interaction problem.

Keywords: wave propagation; Monte Carlo simulation; attenuation coefficient; scattering; modelling.

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1 introduction

To understand the mechanisms and properties of wave propagations and wave-object interaction has significant meanings. It has been a question of growing concern among academia in many medical applications (Cheong et al., 1990). For decades, although there are various modelling to try to simulate the wave propagation and interaction procedures, the Monte Carlo (MC) method has become an important choice for wave transport simulations (Prahl et al., 1989).

The Monte Carlo simulation modelling was first proposed by Metropolis and Ulam. In their modelling, a statistical model was investigated to simulate physical processes (Metropolis and Ulam, 1949). Since then, the Monte Carlo method has been used in various applications, including a very large application code package developed by Los Alamos (Forester and Godfrey, 1985; Briesmeister; 1986). In this large-scale Monte Carlo simulation modelling, detailed neutron and photon physics models that contain the up-to-date cross-sections and reaction information were used. In 1991, Andreo (1991) reported the comparison between the large-scale Monte Carlo simulations with numerous list of applications. For light wave propagations, owing to its flexibility and recent advances, the Monte Carlo simulation has been viewed as the gold standard to model light transport in objects such as tissues (Zhu and Liu, 2013; Skipetrov and Chesnokov, 1998; Farrell et al., 1992). Both forward and inverse problems in tissue optics can be simulated by Monte Carlo method by utilising experimentally measured physical properties values in the wave propagation and interaction (Zhu and Liu, 2013).

In this paper, a Monte Carlo simulation modelling is developed to simulate the light wave transport and interaction with objects including tissues. The formulas necessary for the computer simulation was investigated and described. The general procedure of tracking an individual photon packet, the wave-object interactions were simulated based on the wave absorption and scattering models. Results demonstrate that this Monte Carlo model of wave propagation is capable to simulate the wave transport procedures. It serves as an essential component for our further study of wave propagations and computations.

2 Materials and methods

Wave propagation in tissues is simulated by tracing the random work steps of each photon packet in our MC simulation, based on statistical modelling. In this paper, we focus on light wave propagation as simulation experiments. As a type of electromagnetic radiation, light wave follows the electromagnetic radiation rules of absorption and scattering when it travels through the object.

When the energy level of light waves are high enough, they can have potentials of penetrating objects with attenuation. During the attenuation procedures, different types of interactions may happen. The attenuation coefficient characterises the attenuation property when a beam interacts with an object. Generally speaking, interactions may result in the local deposition of energy. Photons may change directions or shown annihilation.

In order to simulate the light wave propagation, individual photon histories were traced in our MC modelling. The statistics of a large photon population sample was taken into account to achieve accurate estimates of expected results. In this paper, in order to focus on particle characteristics of the light wave in simulation, photons are considered as classical particles, and phases or polarisation are not traced (Prahl et al., 1989; Zhu and Liu, 2013).

Figure 1 shows the flow chart of our MC modelling of the propagation of a single photon packet. The MC modelling of light wave propagation in our simulation involves several steps (Welch et al., 1997; Swartling et al., 2003; Prahl et al., 1989).

A general MC simulation to simulate light wave propagation with optical properties at specific wavelength is implemented first. The photon is generated and then moved with certain steps. Absorption or scattering conditions are calculated and boundary situations are taken into account.

In our MC simulation, a three-dimensional tissue model was used as the object in the *x*-*y*-*z* coordinates space. A photon is launched into the tissue model as the beginning step of MC simulation. The photon's initial direction is chosen according to the simulated incident projection direction from collimated beam. Rather than collimated beam directions, random photon directions can also be generated if the simulation is based upon the diffuse irradiance. In order to approach desired accuracy of the MC computation, variance reduction techniques are implemented to reduce the number of photons (Kalm and Harris, 1951; Prahl et al., 1989). In order to improve the computation efficiency of MC simulation, a packet of photons along each pathway is simulated to propagate in the tissue slab. Some portions of the photons packet will be absorbed, some will be scattered. The size of the photon packet is defined as weight with an initial value of unity in the MC simulation (Prahl et al., 1989).

Each photon is then propagate with an incremental step size of s, which is small compared to the path length of a photon in the tissue slab. The step size is calculated by:

$$s = -\frac{\ln(\varepsilon)}{\mu_a + \mu_s}$$

where ε represents a random number within a range of zero through unity. μ_a is the absorption attenuation coefficient, μ_s is the scattering attenuation coefficient. Therefore, the step size s can be determined. If the step size is too small, the MC computation efficiency will be influenced. If the step size is too large, the approximation of MC simulation will be poor-conditioned. One can also choose to have a varied step size for each photon step. Beer's law should be followed to determine the probability density function for the step size (Prahl et al., 1989).

After initialisation, the photon will be moved with step size during the simulation. Positioning parameters including *x*-*y*-*z* spatial coordinates and direction angles in travel are calculated. The following calculations are used to move the photon:

$$x' = x + \mu_x \cdot s$$
$$y' = y + \mu_y \cdot s$$
$$z' = z + \mu_z \cdot s$$

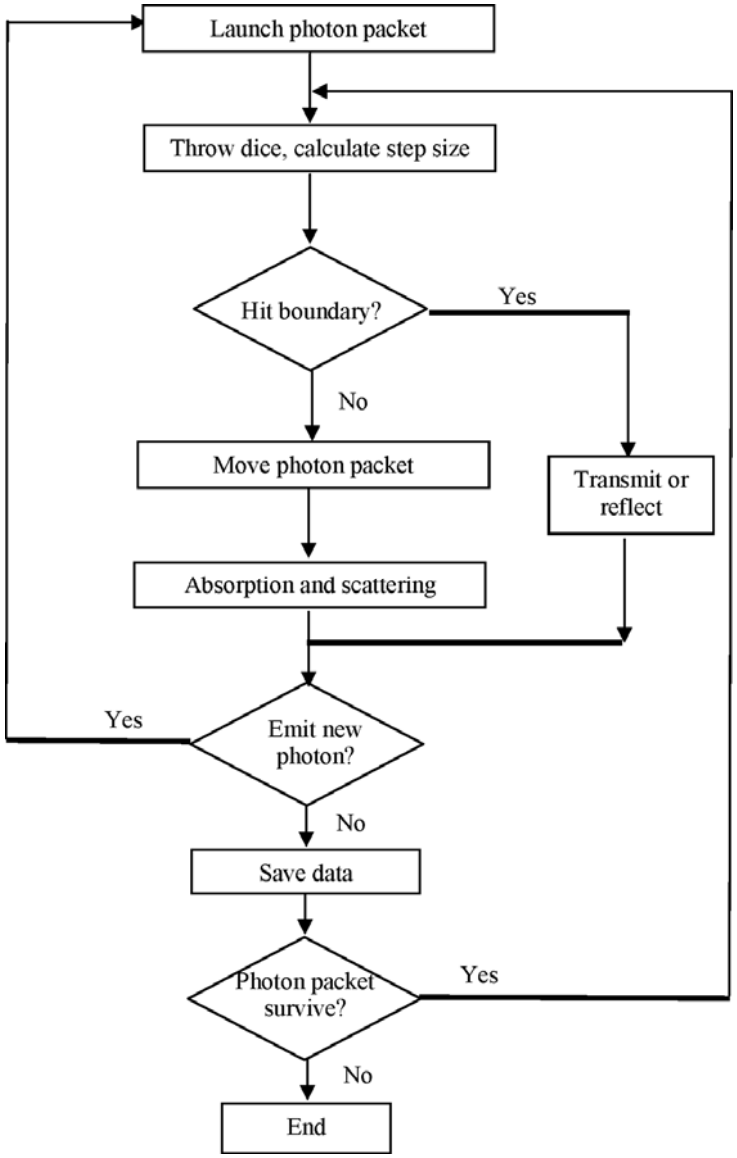
where x, y, z represent the photon location before move. (x', y', z') is the photon new location after move. μ_x, μ_y, μ_z are the *x*-*y*-*z* direction cosines that are specified by taking the cosine of the angle that the photon's direction makes with each axis (Prahl et al., 1989). Boundary conditions are taken into consideration. If a boundary is hit, transmission or reflection will be computed.

If single photon is scattered, the azimuthal angle $\phi = 2\pi\varepsilon$ and the deflection angle will be calculated for each scattering step, and the new x, y, z directional position will be calculated as well. The scattering in tissue can be characterised by the Henyey-Greenstein phase function (Jacques et al., 1987):

$$\cos\theta = \frac{1}{2g}\left\{1+g^2-\left[\frac{1-g^2}{1-g+2g\varepsilon}\right]^2\right\}$$

where θ represents the deflection angle. ε is a random number within a range of zero through unity. g is the anisotropy tissue factor with a typical value of 0.5 to 0.99 for optical properties.

Figure 1 Flow chart of our MC modelling of the propagation of a single photon packet



The new μ_x, μ_y, μ_z of the travelling directions can be calculated by those angles and former information as below:

$$\begin{cases} \mu_x' = \dfrac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_x\mu_z\cos\varphi - \mu_y\sin\varphi) + \mu_x\cos\theta \\ \mu_y' = \dfrac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_y\mu_z\cos\varphi + \mu_x\sin\varphi) + \mu_y\cos\theta \\ \mu_z' = -\sin\theta\cos\varphi\sqrt{1-\mu_z^2} + \mu_z\cos\theta \end{cases}$$

If the angle is very close to the normal, here we use $|\mu_z| > 0.999$, the following formulas are used to calculate the new direction:

$$\begin{cases} \mu_x' = \sin\theta\cos\varphi \\ \mu_y' = \sin\theta\sin\varphi \\ \mu_z' = \dfrac{\mu_z}{|\mu_z|}\cos\varphi \end{cases}$$

The scattering path for each step is recorded in a matrix. If single photon is absorbed after certain steps, the absorption positions are recorded in another matrix. Finally, the photon is killed if the photon termination conditions meet.

3 Results

In our MC simulation, near infrared case is simulated with $\lambda = 1$ μm. Difference attenuation coefficients are used in the model. For an instance, if $\mu_a = 0.2$ cm^{-1}, $\mu_s = 50.2$ cm^{-1}, that is: $l_a = 1/\mu_a = 5$ cm, $l_s = 1/\mu_s = 200$ cm for parameters of absorption and scattering. These parameters are values approximate for human breast tissue at $\lambda = 1$ μm. So we can calculate the $\mu_t = \mu_a + \mu_s$ accordingly. The anisotropy g=0.95 is used for experiment and validation purposes. When weight is smaller than 0.001, the step is discarded and the photon is terminated in this model. In our experiments, 150 photons are used in the model.

Figure 2 shows our simulation example with $\mu_a = 2$ cm^{-1}, $\mu_s = 50$ cm^{-1}. For each photon, the final absorption position is marked by '*' symbol in Figure 2. The original starting position of $x = y = z = 0$ is marked by '*o*' symbol. When the absorption attenuation coefficient is bigger, the maximum absorption path along z axis will be smaller. In Figure 2, the maximum absorption path is only 0.1764 cm, where the mean scatter path is about 113 μm. The attenuation coefficients are inversely proportionally to the mean-free path for absorption and scattering respectively.

The parameter g determines certain scatter characteristics. If $g = 0$, it means the isotropic scattering. If $g = 1$, the completely forward scattering happens. In our illustrated results, the $g = 0.95$ is used for human breast tissue simulation experiments at $\lambda = 1$ μm. One can see that the scattering direction is almost along z axis, due to the relatively large g of 0.95. If we change the g parameter to be smaller, the scattering direction will be more isotropic.

Figure 3 shows the absorption position with $\mu_a = 0.2$ cm^{-1}, $\mu_s = 50$ cm^{-1} parameters. The absorption position along z-axis for 150 photons and the histogram of the distribution of those absorption positions is shown in Figure 4 and Figure 5.

Figure 2 MC simulation with $\mu_a = 2$ cm^{-1}, $\mu_s = 50$ cm^{-1}

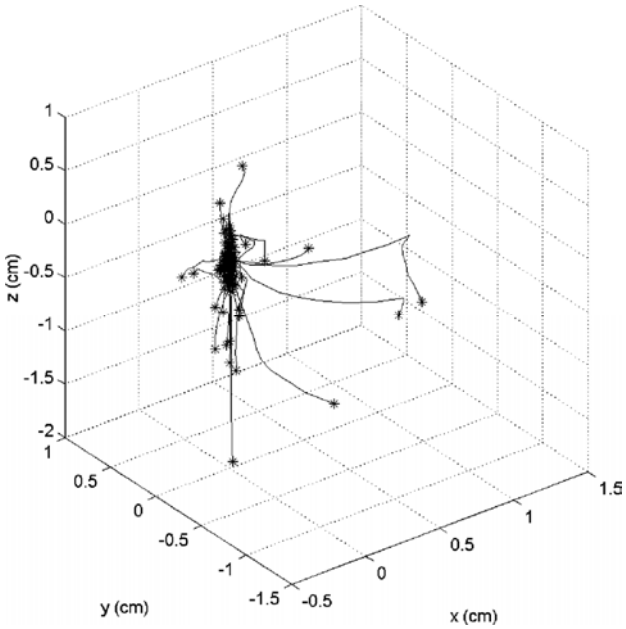


Figure 3 Absorption position for 150 photons

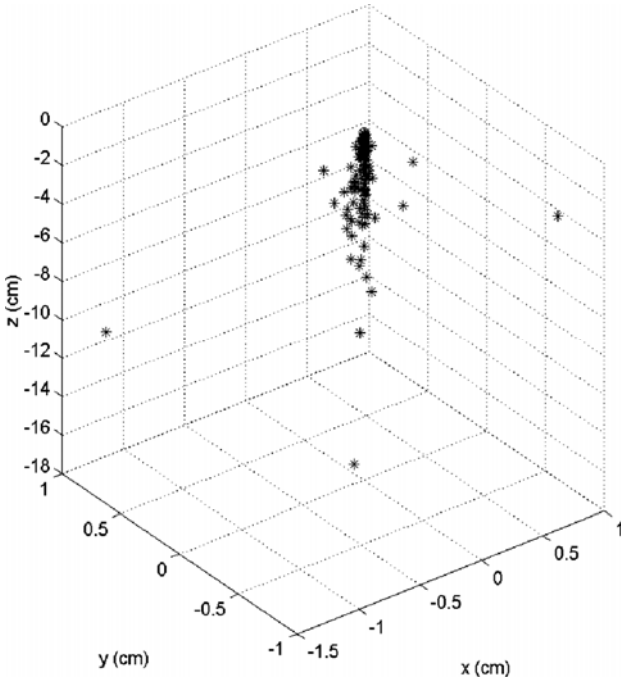


Figure 4 Absorption position along *z*-axis

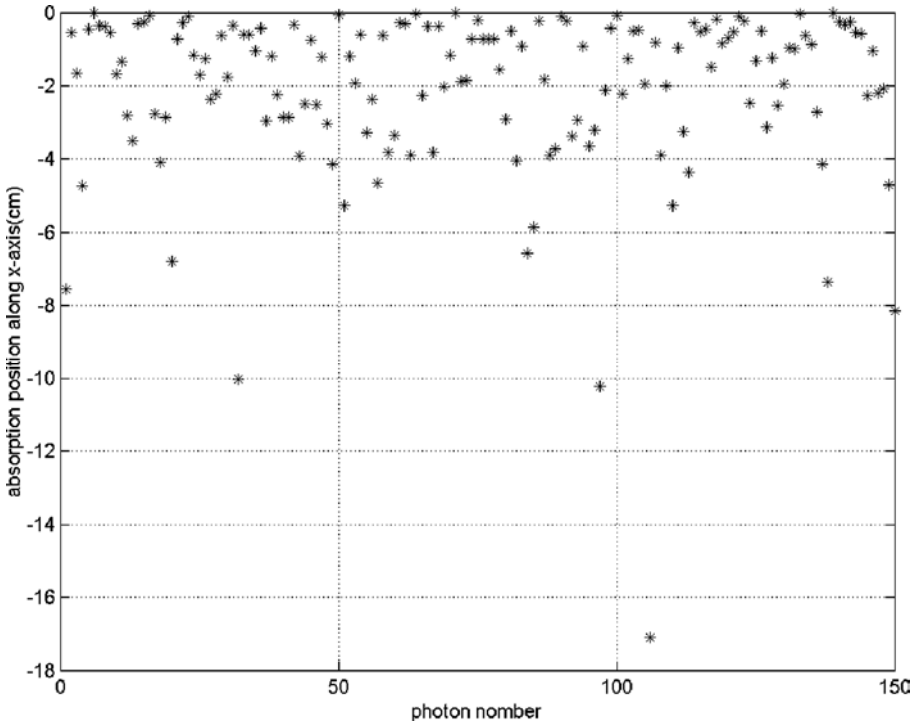
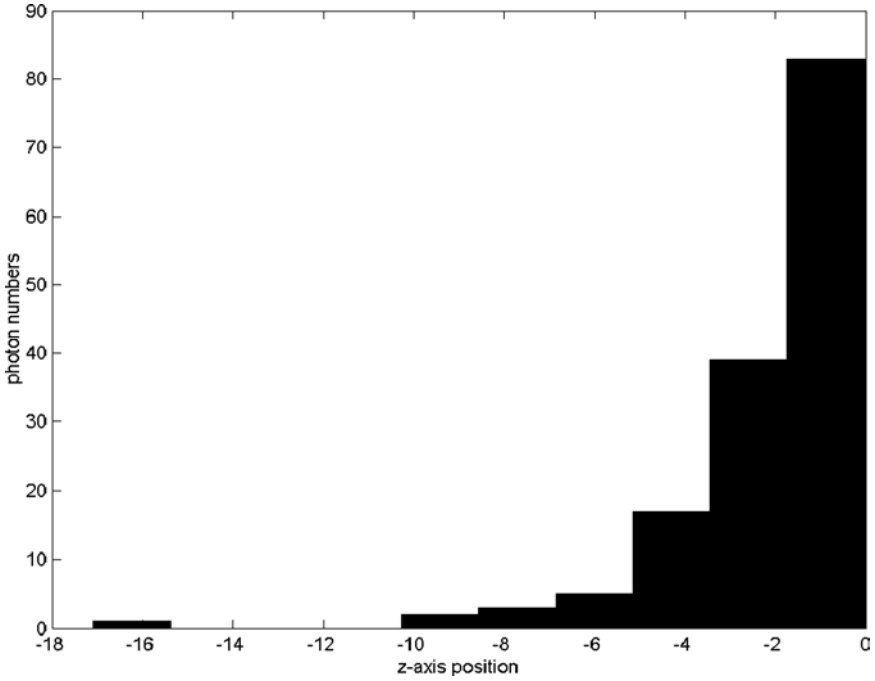


Figure 5 Histogram of the distribution of absorption positions



In Figures 3–5, we assume that the boundary is infinity. When the photon is absorbed finally, the photon will be terminated there. If boundary conditions are added, the internal reflection or transmission condition for photons can be decided too. According to the Fresnel reflection and Snell's law, one can calculate the new direction of photons. With slab geometry, only thickness in the z-direction will be taken into account. The internally reflected photon position is calculated by changing only the z direction of the photons. The μ_z direction will be exactly the opposite of the original z direction. All other x and y direction will be the same as original ones.

4 Conclusion

The MC modelling allows computer simulation of wave propagation and interaction with objects. In this paper, we modelled the photon packets travel of light wave propagation in tissue slabs with various attenuation coefficients. Boundary conditions and anisotropic scattering have been investigated. Several types of light-tissue interactions including absorption and scattering have been simulated the by the MC methods. This work serves as an essential part of our study of optical measurement and wave propagation study. Compared to other non-numerical methods such as diffuse approximation, MC modelling is capable to simulate various illumination and detections. Further work will be done to investigate the MC modelling for wave propagation measurements and instrumentation.

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