A Monte Carlo Model of Light Propagation in Tissue

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ABSTRACT

The Monte Carlo method is rapidly becoming the model of choice for simulating light transport in tissue. This paper provides all the details necessary for implementation of a Monte Carlo program. Variance reduction schemes that improve the efficiency of the Monte Carlo method are discussed. Analytic expressions facilitating convolution calculations for finite flat and Gaussian beams are included. Useful validation benchmarks are presented.

1 Introduction

Monte Carlo refers to a technique first proposed by Metropolis and Ulam to simulate physical processes using a stochastic model.[1] In a radiative transport problem, the Monte Carlo method consists of recording photons histories as they are scattered and absorbed. Monte Carlo programs with great sophistication have been developed—an extreme example is the MCNP Monte Carlo code package at Los Alamos that has involved over 250 person years of development.[2] The Monte Carlo method has been used infrequently to model laser tissue interactions, but these applications have so far neglected anisotropy and internal light reflection.[3]

This paper describes the Monte Carlo method for modelling light transport in tissue. The formulas necessary for implementation of the Monte Carlo method in computer code are provided. This paper discusses internal reflection of a photon at boundaries, shows how the phase function may be used to generate new scattering angles, discusses a few variance reduction schemes to improve efficiency, gives a method for estimating the uncertainty in any Monte Carlo calculation, and gives results for validating the Monte Carlo implementation.

Figure 1 is a flow chart of a Monte Carlo program. Once launched, the photon is moved a distance Δs where it may be scattered, absorbed, propagated undisturbed, internally reflected, or transmitted out of the tissue. The photon is repeatedly moved until it either escapes from or is absorbed by the tissue. If the photon escapes from the tissue, the reflection or transmission of the photon is recorded. If the photon is absorbed, the position of the absorption is recorded. This process is repeated until the desired number of photons have been propagated. The recorded reflection, transmission, and absorption profiles will approach true values (for a tissue with the specified optical properties) as the number of photons propagated approaches infinity.

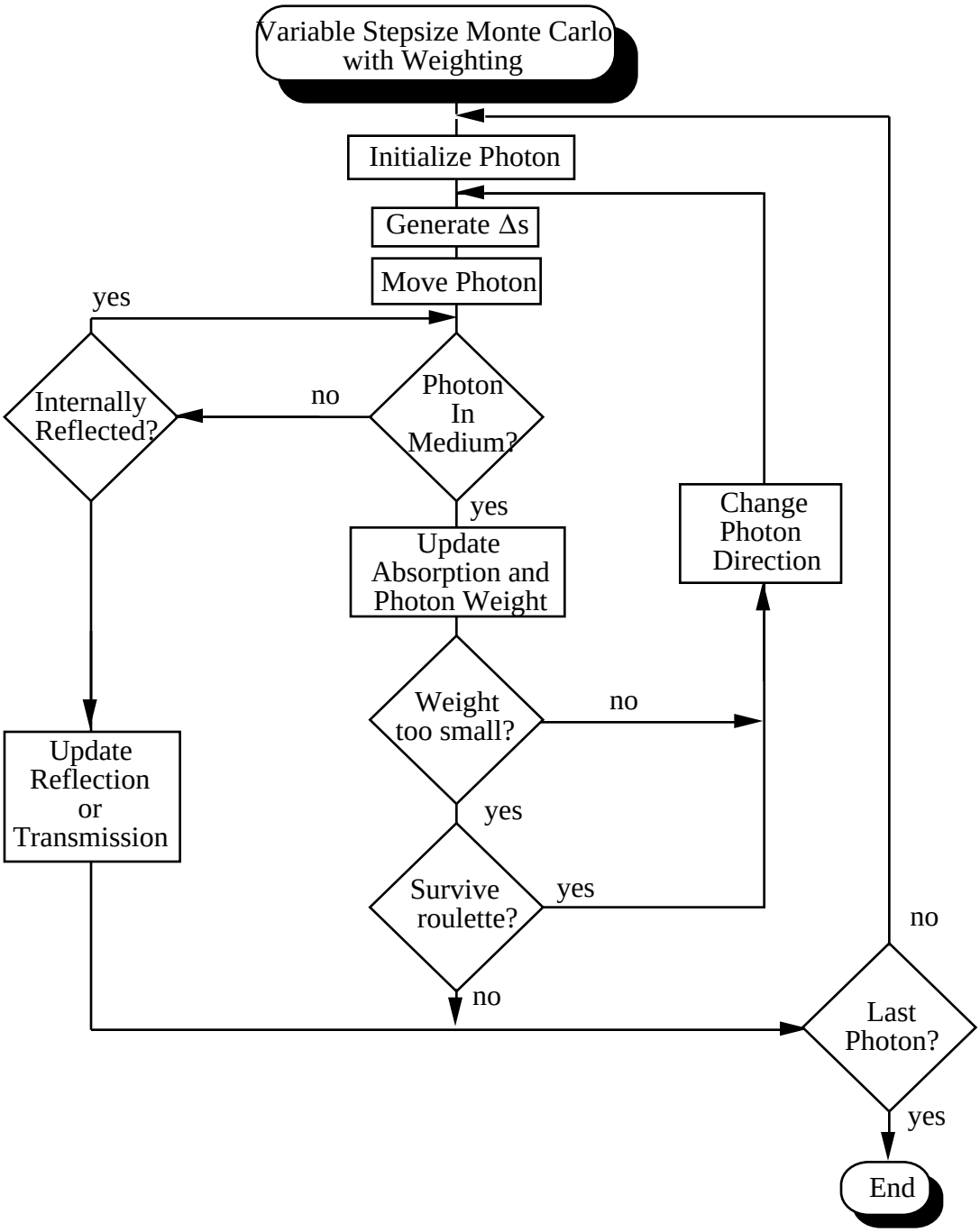

Figure 1: Flowchart for the variable stepsize Monte Carlo technique. The photon packet is initialized. The distance to the first interaction event is found and the photon packet is moved. If the photon has left the tissue, the possibility of internal reflection is checked. If the photon is internally reflected then the photon position is adjusted accordingly and the program continues, otherwise the photon escapes and the event is recorded. For photons which continue, some fraction of the photon packet $(1-a)w$ will be absorbed each step. This fraction is recorded and the photon weight is adjusted. If the weight is above a minimum, then the rest of the photon packet is scattered into a new direction and the process is repeated. If the weight falls below a minimum, then roulette is played to either extinguish or continue propagating the photon. If the photon does not survive the routette, a new photon packet is started.

2 Photon Initialization

The Monte Carlo method begins by launching a photon into the tissue. If a collimated beam normally incident on a slab is simulated then the photon's initial direction is chosen downwards into the tissue. If a diffuse irradiance is simulated, then the photon's direction is chosen randomly from all possible directions in the downward hemisphere. The coordinates of the photon are usually identical for all photons. This allows convolution techniques to be used to determine fluence rates from a wide variety of beam shapes.

Variance reduction techniques are used to reduce the number of photons necessary to achieve the desired accuracy for a Monte Carlo calculation. These techniques have a long history and most important ones were first implemented by Kahn.[4] One simple technique (implicit capture) to improve the efficiency of a Monte Carlo program is to propagate many photons (a packet) along each pathway. Usually only one photon follows each pathway, and at each step the photon may be either absorbed or scattered. If a packet of photons followed each pathway then some portion of the packet would be absorbed at each step. The size of this packet is called the weight (w) of the photon. Its initial weight is set to unity.

3 Generating the Propagation Distance

The simplest Monte Carlo method propagates each photon with small, fixed incremental stepsizes. The fixed stepsize Δs must be small relative to the average mean free pathlength of a photon in the tissue. The mean free pathlength is the reciprocal of the total attenuation coefficient.

$$\Delta s << \frac{1}{\mu_t} = \frac{1}{\mu_s + \mu_a} \tag{1}$$

where μ_t, μ_a, and μ_s are the total attenuation, the absorption, and the scattering coefficients respectively. If the stepsize is too small the photon will rarely interact with the tissue and the Monte Carlo method will be inefficient, conversely if the stepsize is too large then the distanced travelled by a photon is a poor approximation to that of a real photon.

A much more efficient method chooses a different stepsize for each photon step. The probability density function for the stepsize follows Beer's law (i.e. it is more likely for a photon to travel a short distance than a long distance and the probability is proportional to $e^{-\mu_t \Delta s}$.) A function of a random variable (ξ) uniformly

distributed between zero and one which yields a random variable with this distribution is[5]

$$\Delta s = \frac{-\ln \xi}{\mu_t}. \tag{2}$$

The stepsize Δs found using equation (2) represents the distance that a photon will travel before interacting (through absorption or scattering) with the tissue.

4 Moving the photon

A photon is uniquely described by five variables: three spatial coordinates for the position and two directional angles for the direction of travel. However it is convenient to describe the photon's spatial position with three Cartesian coordinates and the direction of travel with three direction cosines.[6] The required formulas for propagation are simple, and the angle variables describing photon direction do not change unless the photon's direction changes. The direction cosines are specified by taking the cosine of the angle that the photon's direction makes with each axis. These are specified by μ_x, μ_y, and μ_z corresponding to each of the x, y, and z-axes respectively. For a photon located at (x, y, z) travelling a distance Δs in the direction (μ_x, μ_y, μ_z), the new coordinates (x', y', z') are given by

$$\begin{aligned} x' &= x + \mu_x \Delta s \\ y' &= y + \mu_y \Delta s \\ z' &= z + \mu_z \Delta s \end{aligned} \tag{3}$$

5 Internal reflection

The possibility of internal reflection occurs when the photon is propagated across a boundary into a region with a different index of refraction. The probability that the photon will be internally reflected is determined by the Fresnel reflection coefficient $R(\theta_i)$

$$R(\theta_i) = \frac{1}{2}\left[\frac{\sin^2(\theta_i - \theta_t)}{\sin^2(\theta_i + \theta_t)} + \frac{\tan^2(\theta_i - \theta_t)}{\tan^2(\theta_i + \theta_t)}\right] \tag{4}$$

where $\theta_i = \cos^{-1} \mu_z$ is the angle of incidence on the boundary and the angle of transmission θ_t is given by Snell's law

$$n_i \sin \theta_i = n_t \sin \theta_t \tag{5}$$

where n_i and n_t are the indices of refraction of the medium from which the photon is incident and transmitted, respectively. A random number ξ uniformly distributed between zero and one is used to decide whether the photon is reflected or transmitted. If $\xi < R(\theta_i)$ then the photon is internally reflected, otherwise the photon exits the tissue and the event is recorded as backscattered light (when the photon exits the top) or transmitted light (when it exits the botton). If the photon is internally reflected, then the position and direction of the photon are adjusted accordingly. For a slab geometry, infinite in the x and y directions with a thickness t in the z-direction, the internally reflected photon position (x'', y'', z'') is obtained by changing only the z-component of the photon coordinates

$$(x'', y'', z'') = \begin{cases} (x, y, -z) & \text{if } z < 0, \\ (x, y, 2\tau - z) & \text{if } z > \tau. \end{cases} \tag{6}$$

The new photon direction (μ'_x, μ'_y, μ'_z) is

$$(\mu'_x, \mu'_y, \mu'_z) = (\mu_x, \mu_y, -\mu_z) \tag{7}$$

and both μ_x and μ_y remain unchanged.

6 Photon absorption

The technique of implicit capture assigns a weight to each photon as it enters tissue. After each propagation step, the photon packet is split into two parts—a fraction is absorbed and the rest is scattered. The fraction of

the packet that is absorbed is

$$fractionabsorbed = \frac{\mu_a}{\mu_a + \mu_s} = 1 - \frac{\mu_s}{\mu_a + \mu_s} = 1 - a \tag{8}$$

where a is the single particle albedo. Consequently, the new photon weight (w') is given by $w' = aw$, which represents the fraction of the packet that is scattered on this step.

An absorption event requires that both the location and the amount of light absorbed be recorded. For example, the appropriate element of the absorption matrix is incremented by $(1 - a)w$. The number of bins in the absorption matrix is determined by the spatial resolution desired. Increasing the number of entries increases the spatial resolution, but also increases the absorption uncertainty in each element (because fewer absorption events will take place in each element and the error is inversely proportional to the square root of the number of absorption events). The fluence rate is obtained by dividing the final value of each matrix element by (1) the equivalent spatial volume of the element, (2) the absorption coefficient, (3) the total number of photons propagated, and (4) the initial weight of each photon.

7 Photon termination

How should the photon (packet) be terminated? Its will never reach zero, and propagating a photon with a minuscule weight yields little information. Absorbing or discarding all the remaining weight, after the weight falls below a minimum (e.g., 0.001), skews the absorption profile or violates energy conservation respectively. A technique called roulette is used to terminate a photon once its weight drops below a specified minimum. The roulette technique gives such a photon (with weight w) one chance in m (e.g., 10) of surviving with a weight mw or else its weight is reduced to zero. The photon is thereby killed in an unbiased fashion, without sacrificing energy conservation and without continuing propagation until its weight has reached zero.

8 Changing photon direction—scattering

A normalized phase function describes the probability density function for the azimuthal and longitudinal angles for a photon when it is scattered. If the phase function has no azimuthal dependence, then the azimuthal angle ϕ is uniformly distributed between 0 and 2π, and may be generated by multiplying a pseudo-random number ξ uniformly distributed over the interval zero to one by 2π (i.e. $\phi = 2\pi\xi$). The azimuthal angle θ for an isotropic distribution is given by

$$\cos\theta = 2\xi - 1 \tag{9}$$

Since scattering in tissue is characterized by the Henyey-Greenstein phase function,[7] the generating function for the Henyey-Greenstein phase function is[5]

$$\cos\theta = \frac{1}{2g}\left\{1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g\xi}\right]^2\right\}. \tag{10}$$

If scattering is isotropic ($g = 0$) then equation (9) should be used.

If a photon is scattered at an angle (θ, ϕ) from the direction (μ_x, μ_y, μ_z) in which it is travelling, then the new direction (μ'_x, μ'_y, μ'_z) is specified by

$$\begin{aligned} \mu'_x &= \tfrac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_x\mu_z\cos\phi - \mu_y\sin\phi) + \mu_x\cos\theta \\ \mu'_y &= \tfrac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_y\mu_z\cos\phi + \mu_x\sin\phi) + \mu_y\cos\theta \\ \mu'_z &= -\sin\theta\cos\phi\sqrt{1-\mu_z^2} + \mu_z\cos\theta \end{aligned} \tag{11}$$

If the angle is too close to the normal (say $|\mu_z| > 0.99999$), the following formulas should be used

$$\begin{aligned} \mu'_x &= \sin\theta\cos\phi \\ \mu'_y &= \sin\theta\sin\phi \\ \mu'_z &= \tfrac{\mu_z}{|\mu_z|}\cos\phi \end{aligned} \tag{12}$$

to obtain the new photon directions.

9 Calculating observable quantities

Potentially, the fluence rate for any irradiation profile may be obtained by launching photons distributed spatially with a probability density function equal to the irradiation profile. Since many photons must be launched at a fixed point before the random fluctuation of the Monte Carlo process becomes small, launching photons from different places increases the total number of photons which must be launched before statistical errors become negligible. Fortunately, the fluence rate which results from photons launched at a single point corresponds to the Green's function $G(x, y, z)$ for the medium. Since the irradiation source profile is not a function of depth, the convolution is independent of z.

The fluence rate for an arbitrary irradiation profile may be obtained by convolving the Green's function profile with the irradiation source function $S(x, y)$

$$\Phi(x, y, z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x', y', z)S(x - x', y - y')\,dx'dy' \tag{13}$$

where $\Phi(x, y, z)$ is the fluence rate at the point (x, y, z). In cylindrical coordinates, the convolution of a cylindrically symmetric irradiation source $S(\mathbf{r})$ and Green's function $G(\mathbf{r})$ will be cylindrically symmetric. This convolution may be written

$$\Phi(r, z) = \int_0^{\infty} G(r', z)\left[\int_0^{2\pi} S\left(\sqrt{r'^2 + r^2 - 2rr'\cos\theta}\right)\,d\theta\right] r'\,dr' \tag{14}$$

where the fluence rate is also cylindrically symmetric and only depends on the radius r and the depth z. The order of integration may be changed in this expression for the fluence rate. Such an expression would be identical, but has the drawback that the inner integral can no longer be found analytically for a finite flat or Gaussian beam.

A Gaussian source function with a $1/e^2$ radius of R is given by

$$S(r) = S_0 e^{-2(r/R)^2} \qquad S_0 = \frac{2P}{\pi R^2} \tag{15}$$

where P is the total power of the beam. The equation for the fluence becomes[8]

$$\Phi(r,z) = S_0 e^{-2(r/R)^2} \int_0^\infty G(r',z) e^{-2(r'/R)^2} I_0(4rr'/R^2)\, 2\pi r'\, dr', \tag{16}$$

where $I_0(r)$ is the zero order modified Bessel function. Notice that the the original Gaussian shape is multiplied by some modulating function. Since $G(r,z)$ and $e^{-r^2} I_0(r^2)$ decrease monotonically, one expects the final internal fluence profile to be a "washed out" Gaussian profile.

The source function for a flat beam with radius R is

$$S(r') = \begin{cases} \frac{P}{\pi R^2} & \text{if } r' \le R, \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

where P is the total power of the beam. The fluence for a flat beam is

$$\Phi(r,z) = \frac{P}{\pi R^2} \int_0^\infty G(r',z) \Theta(r,r') 2\pi r'\, dr' \tag{18}$$

where $\Theta(r,r')$ is given by[8]

$$\Theta(r,r') = \begin{cases} 1 & \text{if } 0 \le r \le R - r', \\ \frac{1}{\pi} \cos^{-1}\left[\frac{r'^2 + r^2 - R^2}{2rr'}\right] & \text{if } |R - r'| \le r \le R + r', \\ 0 & \text{otherwise.} \end{cases} \tag{19}$$

The advantange of equations (16) and (18) is that the fluence requires only one numerical integration, which is significantly faster than the two-dimensionally numerical integration of equation (13).

10 Verification

Two different comparisons with exact values for testing the Monte Carlo implementation were done. The errors shown are standard errors (i.e. the standard deviations of the mean). These values were obtained by splitting one large Monte Carlo run of say 50,000 photons into ten runs of 5,000 each. The results of these ten runs were averaged and the standard error was computed. For an anisotropic phase function and a slab geometry of finite thickness with index matching, van de Hulst's tables served as a reference for reflection and transmission as a function of angle.[9] The phase function was the Henyey-Greenstein phase function with an average cosine of 0.75. The albedo was 0.9. The slab was two optical depths thick, and index-matched with its environment. Light was uniformly incident normal to the slab. The results for total reflection and total transmission for ten runs of 50,000 photons are

	van de Hulst	Monte Carlo	st. dev.
Total Reflection	0.09739	0.0971	0.0003
Total Transmission	0.66096	0.6616	0.0005

Finding exact solutions for media which are not index matched is difficult, but Giovanelli provides data for a semi-infinite slab with isotropic scattering and an index of refraction mismatch of 1.5 to 1.0.[10] Light is normally incident and the slab has an albedo of 0.9. The values for total reflection for ten Monte Carlo runs of 5,000 photons are

	Giovanelli	Monte Carlo	st. dev.
Total Reflection	0.2600	0.2608	0.0008

11 Conclusions

The Monte Carlo model allows calculation of reflection, transmission, and fluence rates in tissue. Both mismatched boundary conditions and anisotropic scattering have been included, thereby increasing the realism of the model. A variable-stepsize weighted Monte Carlo model has been implemented and validated by comparison with published tables. This Monte Carlo model may be used to calculate fluence rates for finite beams irradiating media with cylindrical symmetry by convolving the impulse response with either flat or Gaussian beam irradiation profiles. Analytic expressions that facilitate such calculations have been presented.

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