Published in final edited form as:

Proc SPIE Int Soc Opt Eng. 2006 January 21; 6139: . doi:10.1117/12.646048.

A Macro-Monte Carlo method for the simulation of diffuse light transport in tissue

Jarod C. Finlay* and Timothy C Zhu

Departments of Radiation Oncology, University of Pennsylvania, Philadelphia, PA

Abstract

The Monte Carlo (MC) method of calculating light distributions in turbid media such as tissue has become the gold standard, especially in complex geometries and heterogeneous tissue. The utility of the MC method, however, is limited by its computational intensity. In an effort to reduce the time needed for MC calculations, we have adapted a macro-Monte Carlo (MMC) method (Neuenschwander, *et al.* 1995, *Phys. Med. Biol.* **40**, 543-574) to the solution of tissue optics problems. Traditional MC routines trace individual photons step-by-step through the tissue. Instead, the MMC approach relies on a data set consisting of spheres in which the light absorbed in each voxel is pre-calculated using a traditional MC routine. At each MMC step, the pre-calculated absorbed light dose in the appropriate sphere, aligned to the current position and direction of the sphere, is recorded in the dose matrix. The position and direction of the photon exiting the sphere are chosen from the exit distribution of the pre-calculated sphere, and the process is repeated. By choosing the size of the pre-calculated sphere appropriately, arbitrarily complex boundary geometries can be simulated. We compare the accuracy and calculation time of the MMC method with a traditional MC algorithm for a variety of tissue optical properties and geometries. We find that the MMC algorithm can increase the speed of calculation by as much as two orders of magnitude, depending on the optical properties being simulated, without a significant loss in accuracy.

Keywords

Monte Carlo; fluence rate; turbid media; diffuse reflectance

1. INTRODUCTION

Over the past several decades, Monte Carlo (MC) simulation has come to be accepted as the gold standard for modeling of light transport in turbid media such as tissue. MC simulations can be made arbitrarily accurate, and need not make any approximations, and are based purely on fundamental properties of the media. The most significant disadvantage of the MC method is its computational intensity, which is many orders of magnitude greater than that of analytical methods. This has led to a number of strategies designed to improve the efficiency of MC simulations¹, many of which have been adapted from the analogous work in the fields of nuclear and radiation physics. In this paper, we present the results of an

*finlay@mail.med.upenn.edu; phone 1-215-615-3795;.

implementation of the Macro Monte Carlo (MMC) method originally developed for simulation of radiation dose deposition during radiation therapy.^{2, 3}

Typical MC methods used for tissue optics simulations trace individual photons or 'photon packets' through many scattering and absorption events. The dimensions of the tissue or region of interest being simulated are often orders of magnitude greater than the scattering mean free path (mfp) in the sample, so each photon is scattered tens or hundreds of times before leaving the sample. The result is a very computationally intensive calculation. The MMC method, in contrast, relies on a pre-calculated sphere of deposited light energy, or 'kugel'.³ At each step, the kugel is superimposed on the sample at the position and direction of the photon being traced, depositing the appropriate light dose. The exit position and direction of the photon is then calculated based on the kugel's exit distribution, and the process is repeated. The advantage of this method is that each step essentially makes use of several thousand photon histories rather than just one. The resulting reduction in the variance of each step more than makes up for the increased computational intensity in the dose recording step.

2. METHODS

Creation of the Kugel

For each set of optical properties, a separate kugel was created. The kugel was calculated using a traditional implicit capture MC algorithm based on that of Prahl¹ in a spherical geometry with non-reentrant boundaries. In the implicit capture Monte Carlo algorithm, photons are launched with weight 1.0 and take steps whose length is chosen from a logarithmic distribution with a mean equal to the total mean free path. At the end of each step, a fraction of the photon weight equal to $(1-a)$ is counted as absorbed, where a is the albedo. The remaining weight (the photon weight times the albedo) is scattered and continues on. The scattering angle is selected from the Henyey-Greenstein scattering phase function.⁴ All the weight absorbed within the sphere is counted toward a two-dimensional dose distribution or dose matrix, whose elements are equally-spaced bins in radial distance r and in $\cos \theta$. This distribution completely characterizes the fluence distribution within the sphere resulting from a pencil beam incident in the $+z$ direction at the center of the kugel. For computational efficiency, we resample the dose in the kugel into 1000 equiprobable bins, recording the radial position and polar angle of each.

In order to implement the MMC method correctly, the photons exiting the kugel must be randomly chosen from a distribution matching that of the true kugel. To accomplish this, we record the position of each exiting photon in spherical coordinates. Because the radial distance is determined by the sphere boundary and the simulation is symmetrical with rotation about the z axis, we need only record the polar angle θ . For computational simplicity, we record the value of $\cos \theta$ rather than θ itself. The θ distribution is broken into 100 bins. In each bin, we record the total weight of exiting photons in addition to their mean exit angle with respect to the z axis and the surface normal at the exit position. For ease of computation in later steps, we re-sample this distribution, computing the centers of 100 equiprobable bins. Within each bin, the center angle and mean exit angle are recorded.

Tracing of Photons

A basic flowchart of our Monte Carlo algorithm is shown in figure 1. The steps unique to the MMC method are shaded. First, the photon's new position is chosen such that it lies on the edge of a kugel situated at the photon's current position and direction. The distribution of positions is informed by the pre-calculated kugel results. Second, the photon's new direction is chosen, again from a pre-calculated distribution. Finally, the deposited dose calculated in the kugel, multiplied by the incident photon weight, is deposited in the medium. The deposited weight is divided into k equal parts, each of which is deposited at the position of a randomly selected dose bin. The determination of k is based on the local relative uncertainty, as described below. The end result is that the photon steps through the medium in kugel-radius steps, as illustrated schematically in figure 2.

For ease of use, we have implemented our Monte Carlo algorithm in a Matlab-based graphical user interface, shown in figure 3.

UNCERTAINTY DETERMINATION—Monte Carlo simulations inherently involve statistical uncertainty as a result of the random nature of the calculation algorithm. It is possible to achieve any desired precision by running an appropriate number of photons through the process. The statistical uncertainty can be estimated by comparing sequential runs. The logical extension of this comparison is to treat each photon as an individual Monte Carlo run. In addition to recording the total dose deposited, we record the total squared dose. The total dose and dose uncertainty in any given voxel are then given by

$$\Delta D = \sqrt{\frac{D \sum d_i^2 - (\sum d_i)^2}{N-1}},$$

respectively, where N is the total number of photons traced, d_i is the dose deposited by each photon. This relation allows the determination of the absolute error at any point in the region of interest of the simulation. The relation is valid regardless of whether the photons are propagated by the traditional or the macro Monte Carlo algorithm. Unlike traditional MC methods, the MMC algorithm allows a tradeoff between speed and efficiency in the dose deposition step. During dose deposition, the absorbed photon weight is divided among k positions within the kugel. The value of k is determined by the uncertainty currently determined at the kugel's current position. If the current uncertainty is very small, the speed of the algorithm can be improved by depositing the entire dose at a single point. When the uncertainty is large, the local dose statistics can be improved by dividing the dose among multiple points. On the assumption that the uncertainty scales according to the square root of the number of points sampled, we choose the number of points k to be proportional to the square of the uncertainty.

In our implementation of both the traditional and macro Monte Carlo algorithms, we have implemented the ability to stop the simulation when the maximum uncertainty reaches a preset value. To avoid requiring very low uncertainty in regions of low dose, we count only voxels whose dose is above a pre-defined threshold.

3. RESULTS

Kugel Characteristics

A typical kugel dose distribution, obtained from a simulation with $\mu_a = 0.1 \text{ cm}^{-1}$ and $\mu_s' = 10 \text{ cm}^{-1}$, is shown in figure 4(a). In this case, the dose deposited within the kugel is plotted on a logarithmic scale as a function of angle and radius. Note that the dose is higher in the forward (positive x) direction, indicating that on the scale of the kugel, some anisotropy is retained. In figure 4(b), we plot the exit probability for the same kugel as a function of the cosine of the exit angle. As expected, this distribution is highest at a cosine of 1.0, corresponding to forward propagation. The probability has been normalized to a mean of 1.0.

For computational simplicity, both the exit distribution and the dose distribution are resampled into equiprobable bins. The cumulative probability distributions for exit angle and dose are shown in the left and right panels of figure 5, respectively. In both cases, we plot the simulated distribution (blue) and the approximate distribution resulting from resampling (red).

To be exactly accurate, the distribution of exit angles from the kugel with respect to the kugel normal should be taken into account. It is in principal possible, for instance, for photons exiting at some point on the kugel to preferentially exit in a direction other than normal to the kugel surface. The criterion for exiting the kugel ensures that all photons exiting the kugel must be directed outward. In figure 6, we plot the calculated mean exit cosines with respect to the kugel normal and the incident photon direction as functions of the position on the kugel surface, as given by the polar cosine. The fact that the mean exit cosine shows no position dependence and has a value of approximately 0.75 confirms that the majority of photons leave approximately normal to the kugel surface. Therefore, we position the subsequent kugel normal to the current kugel's surface.

DOSE ACCURACY AND EFFICIENCY—To assess the accuracy of the Macro Monte Carlo method, we have performed a series of paired simulations, one with traditional Monte Carlo simulation and the other with our Macro Monte Carlo algorithm. In each set, the optical properties, source geometry, and criteria for finishing the simulations are the same. For simplicity, we investigated 1-dimensional spherical geometry with an isotropic source at the center. No boundaries were included in the simulation. In figures 7 and 8, we compare the results of the two methods for a series of different optical properties. In each case, the simulated fluence distributions (left panel) are in agreement with one another, and in approximate agreement with the results of an analytic diffusion theory calculation. The disagreement between the Monte Carlo and diffusion theory results near the source are due to the known inaccuracy of the diffusion theory. As shown in the right panel of each figure, the difference between the two Monte Carlo methods is on the order of the uncertainty in the calculations.

When the calculated uncertainty in each simulation reached the predetermined value (5% in this case) at all point above the threshold level, the simulation was stopped, and the total

time and number of photons were recorded. The results are summarized in table 1. The increase in efficiency using the Macro Monte Carlo algorithm is as high as 300 times.

4. DISCUSSION AND FUTURE WORK

In traditional Monte Carlo algorithms, each photon is traced through many steps. Each step involves calculation of the photon's new direction of propagation, new weight, new position, and the bin in the dose matrix to which it corresponds. The computational intensity of the process results from the fact that each of these calculations must be performed tens or hundreds of times per photon, and a typical simulation involves many thousands of photons. The Macro Monte Carlo method involves similar steps, with comparable computational demand, during its propagation. Its computational efficiency gain is due primarily to the fact that far fewer steps are needed to propagate each photon. For this to be true, it is necessary that the kugel be much larger than the mean free path of the photon in the medium. If the kugel is only slightly larger than the photon mean free path, the number of kugel steps needed to propagate a photon will be approximately the same as the number of traditional photon steps, so there will be little gain in efficiency. Conversely, if the kugel is many mean free paths in radius, far fewer kugel steps than traditional steps will be required.

For the algorithm presented here to be generally applicable, it must be capable of taking into account surfaces and boundaries separating tissues of differing optical properties. Because the precalculated kugel assumes homogenous optical properties, it cannot be used in these regions. This difficulty can be avoided by calculating the distance to the nearest boundary at each step in the iteration; If the distance is smaller than the kugel radius, the algorithm can revert to single photon tracing mode (the left branch in figure 2). The checking of boundary distance, however, will become increasingly computationally intensive with increasing complexity of boundaries. Neuenschwander and Born² have avoided this problem by precalculating a matrix of the distance of each point to the nearest boundary, replacing the calculation with a table lookup. Additional efficiency may be gained by allowing multiple kugel sizes to be used, implementing at each step the largest permissible kugel at each point. It should be noted that, while maintaining a library of various sized kugels will increase the needed storage space, it will not significantly increase the time required to produce the kugels, since the calculations needed to precalculate a small kugel are a subset of those needed to calculate a large one.

Acknowledgments

This work was supported in part by Department of Defense grant DAMD17-03-1-0132, NIH PO1 grant CA87971, and NIH R01 grant CA109456.

References

1. Prah SA, Keijzer M, Jacques SL, Welch AJ. A Monte Carlo model of light propagation in tissue. SPIE Institute Series. 1989; IS5:102–111.
2. Neuenschwander H, Born EJ. A macro Monte Carlo method for electron beam dose calculations. Phys Med Biol. 1992; 37:107–125.
3. Neuenschwander H, Mackie TR, Reckwerdt PJ. MMC--a high-performance Monte Carlo code for electron beam treatment planning. Phys Med Biol. 1995; 40:543–574. [PubMed: 7610114]

4. Henyey IG, Greenstein JL. Diffuse radiation in the galaxy. *Astrophys J.* 1941; 93:70–83.

Figure 1.
Flowchart illustrating the steps in a combined implicit capture Monte Carlo and macro Monte Carlo algorithm.

Figure 2.
Schematic representation of the tracing of a single photon *via* the traditional Monte Carlo method (left) and the Macro Monte Carlo method (right)

Figure 3.
Graphical User Interface (GUI) used for running the traditional and Macro Monte Carlo algorithms.

Figure 4.

(a) Deposited dose distribution within a kugel. Optical properties are $\mu_a = 0.1$, $\mu_s' = 10 \text{ cm}^{-1}$. The fluence is plotted in log scale. (b) Exit distribution as a function of polar angle on the kugel surface for the same dose kugel. The cumulative escape probability is 0.200

Figure 5.

Resampling of the simulated exit cosine distribution (left panel) and dose distribution (right panel) as calculated by Monte Carlo simulation in the kugel (symbols) into equiprobable bins(lines).

Figure 6.

Mean angle of the exiting photon with respect to the incident photon (diagonal data set) and the kugel normal (horizontal data set).

Figure 7.

(Left panel) Fluence rate distribution resulting from an isotropic source in an infinite medium, calculated by standard and macro Monte Carlo methods. Optical properties are $\mu_a = 1$, $\mu_s' = 10 \text{ cm}^{-1}$. The fluence is plotted in log scale. The analytic diffusion theory solution is plotted for comparison. (Right panel) The percent difference between the MC and MMC calculations. The calculated uncertainty for the two simulations, summed in quadrature, is shown for comparison.

Figure 8.

(Left panel) Fluence rate distribution resulting from an isotropic source in an infinite medium, calculated by standard and macro Monte Carlo methods. Optical properties are $\mu_a = 0.1$, $\mu_s' = 10 \text{ cm}^{-1}$. The analytic diffusion theory solution is plotted for comparison. (Right panel) The percent difference between the MC and MMC calculations, as in figure 7.

Total time and number of photons traced to achieve an uncertainty of 5% at all points with a dose larger than the threshold times the maximum dose. For the MMC runs, the radius of the precalculated kugel is listed.

Table 1

Optical Properties			MC		MMC			Ratio
μ_s (cm ⁻¹)	μ_s' (cm ⁻¹)	Thresh	Time (s)	Photons	r_{Kugel} (cm)	Time(s)	Photons	
0.01	10	10 ⁻⁷	8892	44432	2	113.45	11900	78.4
0.1	10	10 ⁻⁵	6876	3336	2	22.71	1600	302.8
1	10	10 ⁻⁴	13392	691	1	175.2	1655	76.4