

MONTE CARLO SIMULATION OF LIGHT TRANSPORT THROUGH LENS MONTE KARLO SIMULACIJA PROLASKA SVETLOSTI KROZ SOČIVO

Originalni naučni rad / Original scientific paper

UDK /UDC: 535.2:519.6

Rad primljen / Paper received: 5.11.2016

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Keywords

- Monte Carlo method
- photons transport
- propagation
- lenses
- optics

Abstract

A Monte Carlo model of steady state light transport in contact lenses has been coded in ANSI Standard C. The Monte Carlo simulation offers a flexible, yet rigorous approach to photon transport in tissue which can be applied on the lenses as well. The method describes local rules of photon propagation that are expressed as probability distributions. However, the method is statistical and as such relies on calculating the propagation of large number of photons. As a result, this method requires a large amount of computational time. This method is applied on the lenses and the obtained results are presented. The results confirm the possibility for the theoretical prediction of optical properties of materials.

INTRODUCTION

Monte Carlo simulation has been used to solve a variety of physical problems. So far, there is no well-established definition, but there is a tendency to adopt a definition proposed by Lux et al. [1]. A stochastic model is constructed and the expected value of a certain variable (or of a combination of several variables) is equivalent to the value of a physical quantity to be determined. This definition relates to all applications of the Monte Carlo method. Afterwards, the expected value is estimated by the average of multiple independent samples representing the random variable. For the construction of the series of independent samples, random numbers following the distribution of the variable to be estimated are used.

Monte Carlo simulations offer a flexible, yet at the same time rigorous approach to photon transport in tissues and can score multiple physical quantities simultaneously. This method describes local rules of photon propagation that are expressed, in the simplest case, as probability distribution that describes the step size of photon movement between sites of photon-tissue interaction, and the angles of deflec-

Cljučne reči

- Monte Karlo metoda
- transport fotona
- prostiranje
- sočiva
- optika

Izvod

Monte Karlo model stacionarnog stanja prenosa svetlosti kodiran je u ANSI Standardnom C programu. Monte Karlo simulacije nude fleksibilan, ali rigorozan pristup transportu fenomena u tkivima koje takođe mogu biti primenjene na sočiva. Metod opisuje lokalna pravila prenošenja fotona koja su prikazana kao raspodela verovatnoća. Međutim, ova metoda je u prirodi statistička i kao takva oslanja se na izračunavanje prostiranja velikog broja fotona. Kao rezultat, ova metoda zahteva veliku količinu računskog vremena. Ova metoda je primenjena na sočivima i prikazani su rezultati. Dobijeni rezultati potvrđuju mogućnost teorijskog predviđanja optičkih svojstava materijala.

tion in a photon's trajectory when a scattering event occurs. The Monte Carlo method is statistical in nature and as such, relies on calculating the propagation of a large number of photons (e.g. 10^5) by the computer. Due to the reason mentioned above, a large amount of computational time is required, 1-3, 5/.

Depending on the question being investigated, the precision needed and the spatial resolution desired, the number of required photons might be different [2, 3]. For example, to learn the total diffuse reflectance from a tissue of specified optical properties, about 3000 photons can yield to useful results. To map the spatial distribution of photons, $\phi(r,z)$, in cylindrical symmetry problems, at least 10^4 photons are needed to yield to acceptable and reliable answers, and in more complex problems the photons number might exceed 10^5 . Nevertheless, the flexibility of the Monte Carlo method makes a powerful tool.

These simulations are based on macroscopic optical properties that are assumed to extend uniformly over small units of volume. Mean free paths between photon-tissue interaction sites typically range from 10-1000 μm , with 100 μm as typical value in the visible spectrum [1-3, 5, 13/.

The photons are treated as particles which means that polarization and wave phenomenon are neglected. The scattering can be isotropic although the current version does not consider anisotropic media.

Monte Carlo simulations may be used for diagnostic as well as for therapeutic applications of lasers and other optical sources in medicine [12, 13]. For example, the diffuse reflectance simulated by these simulations can be used to deduce optical properties of tissues which may be ultimately used to differentiate cancerous tissue and the normal one.

In the following sections the problem is described, the strategy of photon tracing into the lens and physical quantities scoring is given as well. These sections are followed by results and conclusion sections.

THE PROBLEM AND COORDINATE SYSTEMS

The method used in this paper describes the transport of an infinitely narrowed photon light beam, perpendicularly introduced on a lens. The wide lens is described by the following parameters: the thickness d (cm), the refractive index n , the absorption coefficient μ_0 (cm⁻¹), the scattering

coefficient μ_s (cm^{-1}), and the anisotropy factor g . Although the real lens can never be infinitely wide, it can be so treated on the condition that it is much wider than the spatial extent of the photon distribution.

The absorption coefficient is defined as probability of photon absorption per unit infinitesimal path-length, and the scattering coefficient is defined as probability of photon scattering per unit of infinitesimal path-length. Sometimes the total interaction coefficient μ_t is used and it is the sum of two before mentioned coefficients [12, 13]. As the other coefficients, it represents the probability of photon interaction per infinitesimal path-length of the lens. The anisotropy coefficient is the average of the cosine value of the deflection angle.

Three different coordinate systems are used in the Monte Carlo simulation. A Cartesian coordinate system is used to trace photon movements; a cylindrical coordinate system is used to score internal photon absorption as a function of r and z coordinates; a spherical coordinate system is used for sampling the propagation direction change of a photon packet. In Fig. 1 a basic flowchart of the Monte Carlo method is given.

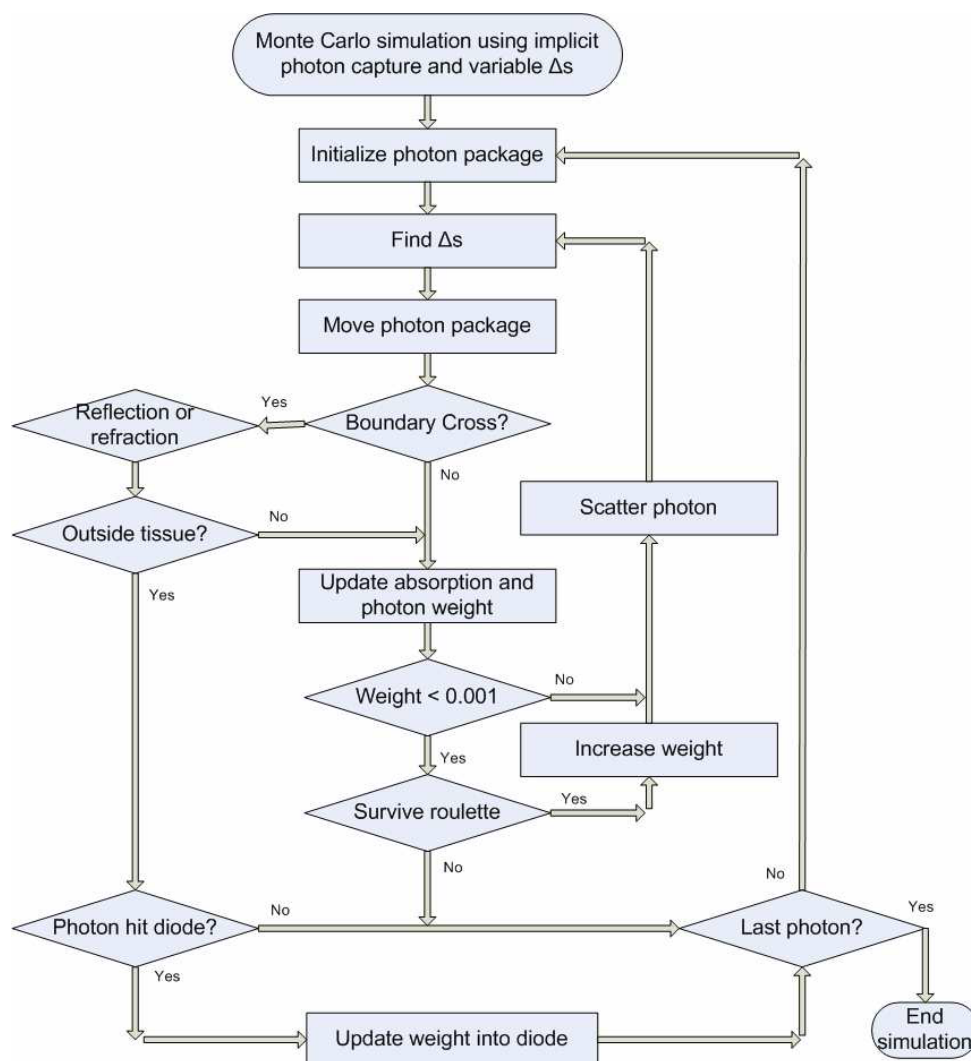


Figure 1. The Monte Carlo simulation flowchart.

SIMULATING PHOTON PROPAGATION

In this section the rules of photon propagation in Monte Carlo simulations are presented. The flowchart presented in Fig. 1 shows basic flow of the photon propagation. Many boxes in the flowchart are a direct implementation of the following discussions and they have been implemented in ANSI Standard C.

Sampling random variables

For random variable χ , there is a probability density function $p(\chi)$ that defines the distribution of χ over the interval (a,b) . The chosen variable may be the angle of deflection that a scattered photon may experience due to the scattering event or the variable step size that photon will take between interactions. For the photon propagation simulation we can choose a value for χ repeatedly and randomly based on a number generator provided by computer. This random variable is created by computer, ε , which is uniformly distributed over the interval $(0,1)$. Non-uniform probability density function $p(\chi)$ can be sampled by solving the following equation, /13/:

$$\int_a^{\chi} P(\chi) d\chi = \zeta \quad (1)$$

Representation of a photon packet

The location of a photon packet described by coordinates (x,y,z) is represented by structure members x, y, z . The structure members ux, uy, uz are representing the travelling directions described by directional cosines (μ_x, μ_y, μ_z) . In order to improve efficiency of the Monte Carlo method, a simple variance reduction technique, implicit photon capture, is used. This technique allows one to equivalently propagate many photons as a packet along a particular pathway simultaneously. A weight, W , is assigned to each photon packet initially. The current weight of the photon packet is denoted by the structure member w , /7, 8, 11/.

The member *dead*, initialized to be 0 when the photon packet is launched, represents the status of a photon packet. If the photon packet has exited the lens or has not survived a Russian roulette (discussed later) when its weight is below the threshold weight, the member *dead* is set to 1. This is used to signal the program to stop tracing the current photon packet.

The step size in dimensionless units, s , is defined as the integration of the interaction coefficient μ_t over the photon pathway. This quantity is known as 'optical distance', and in homogeneous medium the photon path length is multiplied by the interaction coefficient. The number of scatterings experienced by the photon packet is stored in the member *scatters*. The member *scatters* is used to identify the unscattered reflectance or transmittance, or the first interaction inside the lens when photon weight is scored.

A launching of a photon

The photon position is initialized to $(0, 0, 0)$, and the directional cosines are set to $(0, 0, 1)$. The weight is initialized to 1 as well as several other members. When the photon is launched, if there is mismatch between ambient medium (n_1) and the lens (n_2), then the specular reflectance, R_{sp} , will occur, /9-12/.

$$R_{sp} = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} \quad (2)$$

If the lens is between two clear mediums then multiple reflections and transmissions on the two boundaries are considered, and specular reflectance is calculated by:

$$R_{sp} = r_1 + \frac{(1-r_1)^2 r_2}{1-r_1 r_2} \quad (3)$$

where: r_1 and r_2 are the Fresnel reflectances on the two boundaries

$$r_1 = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} \quad (4)$$

$$r_2 = \frac{(n_3 - n_2)^2}{(n_3 + n_2)^2} \quad (5)$$

The photon weight, initialized to 1, is decreased by R_{sp} for the photon packet to enter inside the lens.

$$W = 1 - R_{sp} \quad (6)$$

Equation (3) is used when the system is relatively simple, e.g. system of ambient air and homogeneous lens. Otherwise, the Eq.(4) is used.

Photon's step size

The step size of the photon packet is calculated based on a sampling of the probability distribution for the photon's free path s ($0 \leq s \leq +\infty$). According to the definition of interaction coefficient μ_t , the probability of photon-lens interaction on the interval $(s', s' + ds')$ is:

$$\mu_t = \frac{-dP(s \geq s')}{P(s \geq s') ds'} \quad (7)$$

where: P gives the probability for the condition inside the brackets to hold. After integration of Eq.(7) over interval $(0, s_1)$, exponential distribution is obtained.

$$P(s \geq s_1) = e^{-\mu_t s_1} \quad (8)$$

The probability density function of free path s is:

$$p(s_1) = \frac{dP(s < s_1)}{ds_1} = \mu_t e^{-\mu_t s_1} \quad (9)$$

This equation can be substituted in Eq.(1) which yields to:

$$s_1 = \frac{-\ln(1-\varepsilon)}{\mu_t} \quad (10)$$

Or due to the symmetry:

$$s_1 = \frac{-\ln(\varepsilon)}{\mu_t} \quad (11)$$

This equation is used to sample step size of a photon movement in an infinite or semi-infinite medium. The photon packet which has travelled through $-\ln(\varepsilon)$ will experience a photon-lens interaction. If the interaction occurs, the whole photon packet experience interaction by absorption or scattering. Due to calculation of the logarithmic function, especially for the large number of photons, this method is time consuming. In the literature there are several methods that can be used to alleviate this occurrence.

Photon moving

When sub-step is determined, s_i , the photon is moved in the lens. The newest location is updated in the following manner:

$$\begin{aligned} x_{new} &= x_{old} + \mu_x s_i \\ y_{new} &= y_{old} + \mu_y s_i \\ z_{new} &= z_{old} + \mu_z s_i \end{aligned} \quad (12)$$

Photon absorption

At the time when an interaction site is reached by the photon, a fraction of photon weight (ΔW) is absorbed. This weight will be deposited in the local grid element and can be calculated as:

$$\Delta W = W \left(\frac{\mu_a}{\mu_t} \right) \quad (13)$$

If the photon packet has not been scattered, the photon weight ΔW is scored into the array for the first photon-lens interactions. Otherwise this weight is scored into $A(r, z)$ at the local grid element.

The photon weight has to be updated by:

$$W_{new} = W_{old} - \Delta W \quad (14)$$

Photon scattering

By the time when the photon packet has reached the interaction site and its weight decreased, the photon packet with updated weight is ready to be scattered. To find the direction into which the photon is scattered into, two angles have to be known: the azimuthal angle and the deflection angle. The azimuthal angle, $\psi(0, 2\pi)$ is not dependent on the lens' properties and it can be calculated as:

$$\psi = \cos(2\pi\epsilon) \quad (15)$$

The deflection angle, $\theta(0, \pi)$, however, depends on the optical properties of the lenses, especially the anisotropy determined by the anisotropy factor, $g(-1, 1)$. For lenses this factor is usually approx. 0.9, for light in near infrared range. This means that scattering approaches Mie-scattering which is mainly forward directed. If $g = 0$ the tissue anisotropic properties and probability of the scattering angle is uniformly distributed between 0 and π . If g is negative then mostly backward scattering occurs. The probability density function of the deflection angle can be described by the Henyey-Greenstein phase equation, originally intended for galactic light scattering [5, 6]. The Henyey-Greenstein equation gives the following:

$$p(\cos \theta) = \frac{1 - g^2}{2(1 + g^2 - 2g \cos \theta)^{3/2}} \quad (16)$$

where: g equals $\cos \theta$ is the anisotropy factor and has a value between -1 and 1 . Values of g range between 0.3 and 0.98 , and quite often g is 0.9 in the visible spectrum. By applying Eq.(1), $\cos \theta$ can be expressed as a function of a random number ζ .

The probability function $p(\theta)$ is depicted on Fig. 2. The probability is given as a function of deflection angle for different anisotropy factor. On Fig. 2, a straight horizontal

line indicates isotropic scattering ($g = 0$). As the value of anisotropy factor rises to 1 , the curve is being narrowed with the higher maximal value. A value for g near 1 indicates forward-directed scattering. It was experimentally determined by Jacques et al., that the Henyey-Greenstein function describes single scattering in tissue very well.

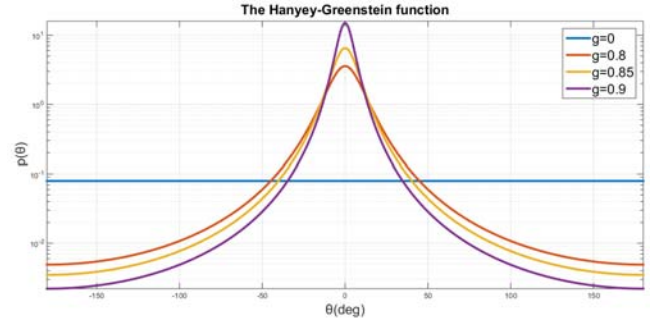


Figure 2. The Henyey-Greenstein function for different values of anisotropy factor, /2-4, 6/.

If $g \neq 0$ then:

$$\cos \theta = \frac{1}{2g} \left\{ 1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g\zeta} \right]^2 \right\} \quad (17)$$

or if $g = 0$ then

$$\cos \theta = 2\zeta - 1 \quad (18)$$

The azimuthal angle, which is uniformly distributed over the interval 0 to 2π , is calculated by:

$$\psi = 2\pi\zeta \quad (19)$$

The newest direction can be calculated with the deflection and azimuthal angles via:

$$\begin{aligned} \mu'_x &= \sin \theta \frac{\mu_x \mu_z \cos \psi - \mu_z \sin \psi}{\sqrt{1 - \mu_z^2}} + \mu_x \cos \theta \\ \mu'_y &= \sin \theta \frac{(\mu_y \mu_z \cos \psi + \mu_x \sin \psi)}{\sqrt{1 - \mu_z^2}} + \mu_y \cos \theta \\ \mu'_z &= -\sin \theta \cos \psi \sqrt{1 - \mu_z^2} + \mu_z \cos \theta \end{aligned} \quad (20)$$

When the photon packet is sufficiently close to the z -axis (e.g. $|\mu_z| > 0.99999$), the next set of the equations should be used, [13, 14],

$$\begin{aligned} \mu'_x &= \sin \theta \cos \psi \\ \mu'_y &= \sin \theta \sin \psi \\ \mu'_z &= \text{sign}(\mu_z) \cos \theta \end{aligned} \quad (21)$$

The function 'sign' returns 1 when μ_z is positive. Otherwise returns -1 if the value is negative.

Reflection or transmission at boundary

During a step, the photon packet may hit a boundary of the lens, which is between the lens and ambient medium. For example, the photon packet may attempt to escape the lens at the interface. If this is the case, it may either escape as observed reflectance or be internally reflected by the boundary. There are several methods of dealing with the photon packet hitting the boundary problem.

Step 1: Computing the distance between current photon location and boundary of the current layer, depending on μ_z :

$$a. \text{ If } \mu_z < 0: \quad d_b = (z_0 - z) / \mu_z \quad (22a)$$

$$b. \text{ If } \mu_z = 0: \quad d_b = \infty \quad (22b)$$

$$c. \text{ If } \mu_z > 0: \quad d_b = (z_1 - z) / \mu_z \quad (22c)$$

where: z_0 and z_1 are the z coordinates of the upper and lower boundaries of the current layer.

Step 2: Decision whether the step size s is greater than d_b . This is done by using equation:

$$d_b \mu_t \leq s \quad (23)$$

If Eq.(23) holds, the photon packet will hit a boundary, and we move the photon packet to the boundary and update s . If Eq.(23) does not hold, the step will fit in the current layer and we move the photon packet to the interaction site where it must experience absorption and scattering.

Step 3: The probability of a photon packet being internally reflected is calculated if it hits the boundary. This probability depends on angle of incidence, α_i , computed by:

$$\alpha_i = \cos^{-1}(|\mu_z|) \quad (24)$$

Snell's law indicates the relationship between the angle of incidence (α_i), the angle of transmission (α_t), and the refractive indices of the media that the photon is incident from (n_i), and transmitted to (n_t):

$$n_i \sin \alpha_i = n_t \sin \alpha_t \quad (25)$$

If $n_i > n_t$, it means that α_i is greater than the critical angle, the internal reflectance $R(\alpha_i)$ is set to 1. Otherwise, $R(\alpha_i)$ is computed by Fresnel's formulas:

$$R(\alpha_i) = \frac{1}{2} \left[\frac{\sin^2(\alpha_i - \alpha_t)}{\sin^2(\alpha_i + \alpha_t)} + \frac{\tan^2(\alpha_i - \alpha_t)}{\tan^2(\alpha_i + \alpha_t)} \right] \quad (26)$$

Because of the assumption made earlier, that light does not have particular polarization, Eq.(26) represents an average reflectance for two orthogonal polarization directions.

Step 4: Determination whether the photon is internally reflected or transmitted, is done by generating a random number ζ , and comparing the random number with the internal reflectance.

If $\zeta \leq R(\alpha_i)$ then the photon is internally reflected.

If $\zeta > R(\alpha_i)$ then the photon transmits.

If the photon is internally reflected, the photon packet stays on the boundary and its directional cosines must be updated by reversing the z component ($\mu_x, \mu_y, -\mu_z$). Then, go to the Step 1.

If the photon packet transmits across the boundary, it might enter another layer of the lens or ambient medium. If the photon packet is transmitted to the next layer of the lens, it must continue propagation with an updated direction computed by:

$$\begin{aligned} \mu_x^i &= \mu_x \frac{\sin \alpha_t}{\sin \alpha_i} \\ \mu_y^i &= \mu_y \frac{\sin \alpha_t}{\sin \alpha_i} \\ \mu_z^i &= \text{sign}(\mu_z) \cos \alpha_i \end{aligned} \quad (27)$$

Or by employing Snell's law:

$$\begin{aligned} \mu_x^i &= \mu_x \frac{n_i}{n_t} \\ \mu_y^i &= \mu_y \frac{n_i}{n_t} \\ \mu_z^i &= \text{sign}(\mu_z) \cos \alpha_i \end{aligned} \quad (28)$$

Afterwards, go back to Step 1 for the next sub-step of propagation.

The photon weight is scored into diffuse reflectance or transmittance when photon packet escapes the lens. If the photon packet has not been scattered, the photon weight is scored into unscattered reflectance or transmittance depending on where the photon packet escapes. If the photon packet has been scattered at least once, the diffusive reflectance, $R_d(r, \alpha_i)$, or diffuse transmittance, $T_d(r, \alpha_i)$, at the particular grid element (r, α_i) must be updated by the amount of escaped photon weight, W . If $z = 0$:

$$R_d(r, \alpha_i) = R_d(r, \alpha_i) + W \quad (29)$$

If $z = d$, the bottom of the lens:

$$T_d(r, \alpha_i) = T_d(r, \alpha_i) + W \quad (30)$$

Due to the fact that the photon has escaped, the tracing of the photon is terminated and a new photon may be launched into the lens and traced afterwards.

Photon termination

After a photon being launched, it can be terminated naturally by reflection transmission out of the lens. A photon is terminated if it escapes the lens or if the photon weight decreases below a defined threshold value. If the photon weight is below this threshold weight (e.g. $W_{th} = 0.0001$), the current photon gets a further chance in m (e.g. $m = 10$) for surviving with a weight of mW . The photon is terminated if it does not survive the so-called Russian roulette:

If $\zeta \leq 1/m$, then

$$W = mW \quad (31)$$

else

$$W = 0 \quad (32)$$

This method conserves energy and yet terminates photons in unbiased manner.

SCORED PHYSICAL QUANTITIES

During the Monte Carlo simulation the photon reflectance, transmittance and absorption are being recorded. The last cells in the r and z directions require special attention due to propagation beyond the lens. In this case, the last cells in r and z directions do not indicate the real value at corresponding locations. However, the angle α is always within the bound, $0 \leq \alpha \leq \pi/2$, hence in this manner a problem in the scoring of angular distributions of diffuse reflectance and transmittance is precluded.

Reflectance and transmittance

After launching a photon, the specular reflectance is calculated, and the photon weight is transmitted to the lens. During the simulation, some photons may exit the media

and their weight is scored into diffusive reflectance or diffusive transmittance depending on location where the photon exits. The photon packets are internally represented by two arrays: $R_{d-r\alpha}[i_r, i_\alpha]$ and $T_{d-r\alpha}[i_r, i_\alpha]$ where i_r and i_α are indices for r and α which are in the range: $0 \leq i_r \leq N_r - 1$, $0 \leq i_\alpha \leq N_\alpha - 1$. The coordinates are optimized to minimize error:

$$r = \left[(i + 0.5) + \frac{1}{12(i + 0.5)} \right] \Delta r \quad (33)$$

$$\alpha = (i + 0.5)\Delta\alpha + c \tan((i + 0.5)\Delta\alpha) \times \left[1 - \frac{\Delta\alpha}{2} - c \tan\left(\frac{\Delta\alpha}{2}\right) \right] \quad (34)$$

The values for r are given in (cm) and for α in (rad).

After tracing multiple photon packets N , the raw data $R_{d-r\alpha}[i_r, i_\alpha]$ and $T_{d-r\alpha}[i_r, i_\alpha]$ provide the total photon weight in each grid element. The total photon weight in grid elements in each direction is calculated as follows:

$$R_{d-r}[i_r] = \sum_{i_\alpha=0}^{N_\alpha-1} R_{d-r\alpha}[i_r, i_\alpha] \quad (35)$$

$$R_{d-\alpha}[i_\alpha] = \sum_{i_r=0}^{N_r-1} R_{d-r\alpha}[i_r, i_\alpha] \quad (36)$$

$$T_{d-r}[i_r] = \sum_{i_\alpha=0}^{N_\alpha-1} T_{d-r\alpha}[i_r, i_\alpha] \quad (37)$$

$$T_{d-\alpha}[i_\alpha] = \sum_{i_r=0}^{N_r-1} T_{d-r\alpha}[i_r, i_\alpha] \quad (38)$$

Total diffuse reflectance and transmittance are computed by summation of the 1-D arrays:

$$R_d = \sum_{i_r=0}^{N_r-1} R_{d-r}[i_r] \quad (39)$$

$$T_d = \sum_{i_r=0}^{N_r-1} T_{d-r}[i_r] \quad (40)$$

Total diffuse reflectance and transmittance are divided by the number of photon packets N to compute probabilities:

$$R_d = \frac{R_d}{N} \quad (41)$$

$$T_d = \frac{T_d}{N} \quad (42)$$

Since R_d and T_d are probabilities, they are dimensionless.

RESULTS AND RECOMMENDATIONS

Diffusive reflectance and transmittance are computed for a lens with properties given in the Table below.

Table 1. Properties used in the simulation.

Property	Units	Quantity
Relative refractive index	–	1.47
Absorption coefficient	cm^{-1}	10
Scattering coefficient	cm^{-1}	60
Anisotropy factor	–	0.9
Thickness	mm	0.02

Ten Monte Carlo simulations of 10^4 photon packets each are completed and the total diffusive reflectance and transmittance are averaged and calculated with standard deviation. Results are given below:

$$R_d = 0.04435 \pm 0.00049 \quad (42)$$

$$T_d = 0.94275 \pm 0.00083 \quad (43)$$

Results indicate that about 94% of proton packets are transmitted while 4% are reflected. The rest of about 2% are absorbed by the lens.

The obtained results confirm the possibility for the theoretical prediction of materials optical properties. Optical characteristics of the material are: absorbance, reflectance and transmittance.

Therefore, the advantage of the Monte Carlo simulation is that any parameter, such as the path, absorption position and many others, can be logged. Also, there are not any limitations in lens geometry or homogeneity. The serious drawback is the substantial computational time needed in order to have reliable results. Contrary to this, Monte Carlo is a powerful tool.

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