Scattering Specific Characteristics of Continuous Medium for Monte Carlo Simulations of Light Transport in Turbid Biological Tissues

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Abstract **- Using examples of 1D and 2D pure scattering problems and a single-scattering approximation, the paper considers the derivation of expressions for the scattering coefficient and the phase scattering function for a continuous medium as the limiting case of scattering on a group of discrete scatterers. It is shown that the use of this approach to construct the cumulative distribution function (CDF), which serves to simulate the scattering angle at numerical Monte Carlo simulations, leads to the dependence of CDF only on the normalized scattering phase function of a single scatterer.**

Keywords - Monte Carlo, light transport, scattering, phase function, continuous medium, particles, analytical solution, biological medium

Since there is no exact analytical solution of the transport equation, its various approximations, as well as the Monte Carlo (MC) numerical computational method, are actively used for theoretical investigations of light transport in turbid (scattering) media, biological tissues and media for example. Main scattering elements in a biological tissue are the cells membranes, nuclear membranes and other discrete optical inhomogeneities inside light-absorbing substances. At the same time, both the light transport theory and the MC numerical method operate with continuous media, the optical properties of which should be determined as specific characteristics per a length of a light-beam path.

At MC simulations, it is common to use such optical characteristics of the medium as the refractive index n, absorption and scattering coefficients μ_a and μ_s, and the scattering phase function (SPF) ρ at a single scattering event. With the help of n, the refraction and reflection at boundaries between different turbid media with different optical properties are usually taken into account. Coefficients μ_a and μ_s determine dissipation (absorption and scattering) of radiation inside the medium of light propagation, while SPF ρ determines angular (spatial) distribution of the scattered radiation. In fact, parameters μ_a and μ_s are the specific characteristics of the infinitesimal element dl of the beam path length in the medium, which have a dimension of a reciprocal length [cm^{-1}]. At MC simulations, these coefficients are commonly used to sample both the path length l for every step of simulations of the photon propagation inside the medium, and the scattering probability P_s for the photon at the end of l. In particular, in the classical MC approach it is accepted:

$$l = -\frac{ln\xi}{\mu_a+\mu_s}; \qquad P_s = \frac{\mu_s}{\mu_a+\mu_s}, \tag{1}$$

where ξ is a random number within the interval [0;1].

Such "point" MC calculations look similar to the problem of discrete scatterers, scattering on particles, for example [1]. However, contrary to the classic theory [2], in [3], it was recently shown that for a group of discrete scatterers, μ_s is not equal to a multiplication of the density of scatterers μ_ρ and the integral scattering characteristic of a single scatterer – a reflectivity R. This difference leads to inaccuracies in MC algorithms for scattering and absorbing media right starting from the one-dimensional (1D) problems [4]. The cause is that the path length and the scattering probability (1) were derived under the assumption that absorption and scattering processes are independent, which is not correct in the general case [5]. Therefore, as a continuation of the study, the aim of this paper is to study how to derive correctly a closed-form expression for SPF Φ for scattering and non-absorbing continuous media as the limit case of the discrete scatterers problem.

Initially, we start with the reproduction of the approach implemented in [3] that describes the algorithm to derive a scattering coefficient μ_s for a continuous 1D turbid medium from the density of scatterers μ_ρ and the scattering characteristics of a single scatterer – a Fresnel reflectivity R. The approach can be conveniently shown by the example of a semi-infinite 1D medium without absorption using the single scattering approximation (SSA). It gives the simplest solution of the 1D scattering problem. SSA assumes scattering (more exactly – the back reflection in the 1D case) for the forward flus $F_+(x)$ on each inhomogeneity and the absence of scattering for the backward flux $F_-(x)$, i.e. it assumes the negligible rereflection process between any two heterogeneities inside the medium.

Assume that an external beam of light (flux) F_0 enters the 1D medium from the left side at the point x = 0 (Fig. 1). Define X as the axis of the direction of the light beam propagation inside the medium.

In the case of 1D pure scattering media, there are only a few physical properties of the media – a number of scatterers distributed along the X-axis inside the medium with the density μ_ρ, and the reflectivity R_i for each i-th scatterer. Due

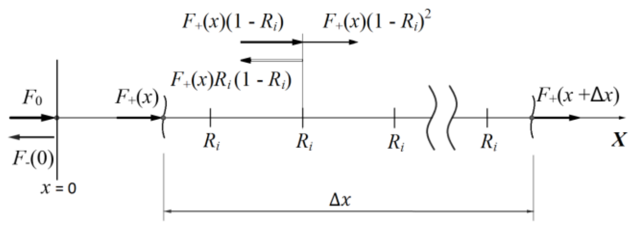

Fig. 1. Outline of the 1D scattering problem without absorption illustrating the structure of the interval Δx. The formation of transmitted and backscattered fluxes is shown through the example of the second scatterer at Δx.

to the absence of absorption, distances between scatterers play no role. Assume all R_i = const ≡ R. For a formation of the scattering coefficient, the difference between them does not matter. To derive differential equations for forward $F_+(x)$ and backward fluxes $F_-(x)$, one need to describe a decrement of the fluxes on dx.

A number of scatterers N inside Δx by a definition is:

$$N = \mu_\rho \Delta x. \tag{2}$$

In addition, by a definition, the derivative for $F_+(x)$ is

$$\frac{dF_+(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta F_+(x)}{\Delta x} = \lim_{\Delta x \to 0} \frac{F_+(x+\Delta x) - F_+(x)}{\Delta x}. \tag{3}$$

Considering partial reflection from each heterogeneity at a point x as $R \cdot F_+(x)$, one can write for $F_+(x+\Delta x)$:

$$F_+(x + \Delta x) = F_+(x)(1 - R)^N. \tag{4}$$

Then, (3) comes to

$$\frac{dF_+(x)}{dx} = F_+(x) \lim_{\Delta x \to 0} \frac{(1-R)^N - 1}{\Delta x}. \tag{5}$$

Finally, taking into account (2), we come to the well-known differential equation for $F_+(x)$:

$$\frac{dF_+(x)}{dx} = -\mu_s F_+(x), \tag{6}$$

where

$$\mu_s = -\mu_\rho \ln(1 - R). \tag{7}$$

Note, that at SSA for 2D and 3D similar theoretical problems, (7) will retain its form, since the absorption and scattering coefficients describe the processes occurring along the light beam propagation path and, strictly speaking, are just the 1D specific quantities.

Along with (6) for the forward flux $F_+(x)$, one can derive the similar equation for $F_-(x)$:

$$\frac{dF_-(x)}{dx} = -\mu_s F_+(x), \tag{8}$$

Thus, when going to a continuous medium, the parameter of scattering, which characterize the scattering process in continuous interval dx, becomes the specific value in the form of $\mu_s \neq \mu_\rho \cdot R$.

Despite the fact that in classic MC algorithms for a turbid continuous medium, the specific characteristics μ_a and μ_s are used to account scattering and absorption, the definition of a new scattering angle is usually carried out with the use of SPF ρ of a single "point" scatterer. As far as we know, the reason for the usage of SPF ρ for continuous media is not explained in details anywhere. However, MC simulations with the use of ρ turns out to be quite accurate. It means that this approach should be very close to the truth.

Phenomenologically, by analogy with μ_a and μ_s, the specific SPF Φ of the infinitesimal element dx of the beam path length in continuous media should exist. Let us try to derive a rigorous equation for it with the use of the above stated approach.

For simplicity, we will consider the same pure scattering problem at SSA. However, any angle scattering leads to at least 2D scattering problem for the pencil-like illuminating beam F_0 (Fig. 2). Usually, the final goal of such task is to find the flux backscattered by the medium through the "window" (detector) of a width w_y located at the Y-axis (similar problem with absorption was considered in detail and solved in [6]), or the flux scattered forward through the similar window in the direction of the beam propagation.

The system of differential equations for this problem is the system (9) [6]. The first equation for the forward flux $F_+(x)$ still remains in the form of (6). The second one describes angular distribution of the flux $F_s(x,\theta)$ scattered on the element dx.

$$\begin{cases} \frac{dF_+(x)}{dx} = -\mu_s F_+(x) \\ \frac{\partial^2 F_s(x,\theta)}{\partial\theta \cdot \partial x} = -\beta_2^+(\theta) F_+(x) \end{cases}, \tag{9}$$

where $\beta_2^+(\theta)$ is the side-scattering coefficient [rad^{-1}·cm^{-1}] that includes the single scatterer's SPF $\rho(\theta)$, and θ is the angle between the direction of the forward flux propagation and a new direction after the scattering event. The closed analytical form of $\beta_2^+(\theta)$ must be phenomenologically determined by how the flux $F_+(x)$ transforms within the element dx.

Formally, the system (9) must contain one more equation – an equation for the radiance propagating back to the medium's boundary (Y-axis) in the direction specified by the angle θ. However, since the pure scattering model considers light propagation inside the non-absorbing medium, as well as SSA considers scattering once along X-axis only, the

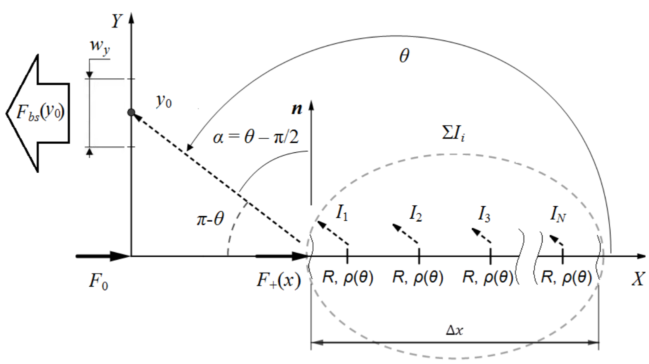

Fig. 2. Outline of the 2D scattering problem without absorption illustrating the structure of the interval Δx and formation of the scattered flux.

radiance will not change along its path, and there is no need in the third equation.

Since the scattered flux in this 2D problem, as well as in the above 1D case, is formed only by the scattered fraction of the forward flux, and there is no absorption inside dx, we can write the following equation at any point x:

$$\int_0^{2\pi} \beta_2^+(\theta) F_+(x) d\theta = \mu_s F_+(x), \tag{10}$$

and, therefore:

$$\int_0^{2\pi} \beta_2^+(\theta) d\theta = \mu_s, \tag{11}$$

which serves as a certain condition when choosing a coefficient $\beta_2^+(\theta)$.

The single scatterer's 2D SPF $\rho(\theta)$ should not be a function of the coordinates x, because all single scatterers in our model are assumed to be equal. In the classic photometry for a point scatterer, $\rho(\theta)$ is determined by the flux F_0 incident on the scatterer and by the radiant intensity of the scattered radiation $I(\theta)$ as follows [7]:

$$\rho(\theta) = \frac{I(\theta)}{F_0}. \tag{12}$$

In our case, it yields:

$$\rho(\theta) = \frac{I(\theta,x)}{F_+(x)}, \tag{13}$$

which has a dimension [rad^{-1}].

In Fig. 2, the structure of the element Δx is the same as in the Fig. 1 for the 1D case. The difference is that in the current problem each scatterer has not only the reflectivity R_i but also SPF $\rho(\theta)$. Using R, we consider nonperfect scatterer (not all incident radiation is scattered), therefore the normalization condition for $\rho(\theta)$ takes place:

$$\int_0^{2\pi} \rho(\theta) d\theta = R. \tag{14}$$

According to (13), dx "generates" (see Fig. 2) a series of radiant intensities $I_i(\theta,x)$, which can be used for determination of 2D SPF $\Phi(x,\theta)$ for continuous dx. For this purpose, first, we will find the sum of these radiant intensities scattered by all scatterers inside Δx in the direction specified by θ. For the first scatterer, the radiant intensity can be written as follows:

$$I_1(\theta,x) = F_+(x)\rho(\theta). \tag{15}$$

For the second one,

$$I_2(\theta,x) = F_+(x)(1-R)\rho(\theta). \tag{16}$$

For the N-th scatterer,

$$I_N(\theta,x) = F_+(x)(1-R)^{N-1}\rho(\theta). \tag{17}$$

The sum of all these radiant intensities can be obtained using the expression for the sum of N terms of a geometrical progression:

$$\sum_{i=1}^{N} I_i(\theta,x) = F_+(x)\rho(\theta)\, \frac{1-(1-R)^N}{1-(1-R)}. \tag{18}$$

With the use of (7), the limit of the ratio of the sum (18) to Δx at $\Delta x \to 0$ gives:

$$\lim_{\Delta x\to 0} \frac{\sum_{i=1}^{N} I_i(\theta,x)}{\Delta x} = \beta_2^+(\theta) F_+(x), \tag{19}$$

where

$$\beta_2^+(\theta) = \rho(\theta) \frac{\mu_s}{1-e^{-\frac{\mu_s}{\mu_\rho}}}. \tag{20}$$

We should note that the consideration of a flux transformation in the way of (15-18) results in $\beta_2^+(\theta)$ that meets the condition (11). This can talk of a correctness of such a consideration.

On the other hand, note that by definition [8],

$$\lim_{\Delta x\to 0} \frac{\Delta I(\theta,x)}{\Delta x} = L(\theta,x)\cdot\cos(\theta - \tfrac{\pi}{2}), \tag{21}$$

where $L(\theta,x)$ is the 2D radiance [W·rad^{-1}·cm^{-1}], and $\theta - \pi/2 = \alpha$ is an angle between the normal $\boldsymbol{n}$ to the element dx at the point $(x,0)$ and the observation direction specified by θ (Fig. 2). Thus, the radiance serves as a specific characteristic of scattering in a continuous medium.

Now, following the classic approach (for example, (12) or (13)), we can define the SPF $\Phi(\theta)$ for a continuous medium as:

$$\Phi(\theta) = \frac{1}{F_+(x)} L(\theta,x)\cdot\sin(\theta), \tag{22}$$

taking into account that $\cos\left(\theta - \frac{\pi}{2}\right) = \sin(\theta)$.

Or, looking at (9), one can write:

$$\Phi(x,\theta) = -\frac{1}{F_+(x)} \cdot \frac{\partial^2 F_s(x,\theta)}{\partial\theta\partial x}. \tag{23}$$

We must notice that the similar expression for 3D SPF is given in [8] and referred there as a volume scattering function (or just a scattering indicatrix).

With the use of (7), (19), (20), (21) and (22) it yields the SPF for non-absorbing 2D continuous media in the form:

$$\Phi(\theta) \equiv \beta_2^+(\theta). \tag{24}$$

Thus, in our model the side-scattering coefficient $\beta_2^+(\theta)$ can be considered as SPF of a continuous medium that turns out to be similar for every point of X-axis for the isotropic scattering medium.

For MC simulations, it is necessary to know the cumulative distribution function (CDF) $D_\theta(\varepsilon)$ that serves for modeling the scattering angle θ (ε is a random number within the range [0; 2π]). Let us build CDF basing on the SPF $\Phi(\theta)$.

The function

$$S(\theta) = \frac{\int_0^{\theta} \Phi(\theta')d\theta'}{\int_0^{2\pi} \Phi(\theta')d\theta'} \tag{25}$$

determines the fraction of the radiation scattered in the angle range [0; θ].

Let us directly map ranges of the definition of the function $S(\theta)$ and CDF $D_\theta(\varepsilon)$ making a model:

$$S(\theta) = D_\theta(\varepsilon). \qquad (26)$$

Since $\int_0^{2\pi} \beta_2^+(\theta) d\theta' = \mu_s$, (26) results in the expression for CDF:

$$D_\theta(\varepsilon) = \frac{1}{\mu_s} \int_0^{k_\theta \varepsilon} \beta_2^+(\theta) d\theta, \qquad (27)$$

where values $k_\theta \cdot \varepsilon$ linearly map the values of θ, because the angle θ itself cannot be treated as a random variable. Therefore, the constant k_θ has the magnitude of 1 rad.

After this, the angle θ can be sampled by the equation

$$\theta = k_\theta D_\theta{}^{-1}(\xi), \qquad (28)$$

where $D_\theta{}^{-1}(\xi)$ is the inverse function to $D_\theta(\varepsilon)$, ξ is a random number uniformly distributed within the range [0;1] and sampled by a computer. When modeling, the constant k_θ can be ignored.

Finally, for the solution of the problem and constructing the corresponding MC model, we need to determine the coefficient $\beta_2^+(\theta)$ in the explicit form like (20).

In [6], it was shown that independently of which $\beta_2^+(\theta)$ is chosen (being subject to only condition $\int_0^{2\pi} \beta_2^+(\theta) d\theta \leq \mu_s$ at SSA), the result of MC simulations always coincides with the analytical solution, as the parameters of the MC model cannot be constructed without the knowledge of this analytical solution. Within this context, the ability of MC simulations to serve us as a reference method to check the correctness of one analytical model or another comes into a question.

From (20) and (24) one can see that $\Phi(\theta)$ is determined not only by SPF of a single scatterer but also by the scattering coefficient μ_s and the reflectivity R.

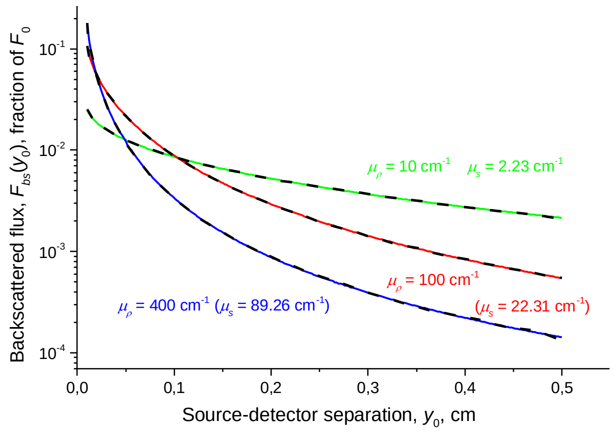

Fig. 2. Dependences of $F_{bs}(y_0)$ on y_0 at different μ_ρ calculated using (30) (solid lines) and MC (dashed lines). The logarithmic scale is used along the ordinate axis. The parameters: R = 0.2, w_y = 0.02 cm, $\rho(\theta)$ = $R/2\pi$. The number of incident photons used in MC is 10^7.

For the case of SSA and non-absorbing media, (27) for CDF of the scattering angle using (7) and (20) comes to

$$D_\theta(\varepsilon) = \frac{1}{R} \int_0^{k_\theta \varepsilon} \rho(\theta) d\theta. \qquad (29)$$

It can be seen from (29) that the scattering angle sampled from (28) is determined *only* by single scatterer's SPF $\rho(\theta)$ and R. Thus, the use of SPF of a continuous medium $\Phi(\theta)$ results in the conventional method of sampling the scattering angle.

Knowing $\beta_2^+(\theta)$, one can obtain the strict analytical solution of the problem, namely, the backscattered flux left the medium through the window of width w_y centered at the point $(0,y_0)$. Taking into consideration the window boundaries $y_1 = y_0 - w_y/2$ and $y_2 = y_0 + w_y/2 \geq 0$, as well as the equation $x = -y/\mathrm{tg}\theta$, one comes to the desired backscattered flux:

$$F_{bs}(y_0) = F_0 \frac{1}{1-\exp(-\mu_s/\mu_\rho)} \int_{\frac{\pi}{2}}^{\pi} \rho(\theta)[\exp(\mu_s y_1/\tan\theta) - \exp(\mu_s y_2/\tan\theta)]\, d\theta. \qquad (30)$$

The function $F_{bs}(y_0)$ for the case of isotropic scattering $\rho(\theta) = R/2\pi$, with the reflectivity R = 0.2 at the window width w_y = 0.02 cm and various scatterer densities μ_ρ (which results in various μ_s) is plotted in Fig. 3. Also, results of the corresponding MC simulations conducted with the use of (29) for CDF and the path length $l = -\ln\xi/\mu_s$ are presented there. One can see no visible differences in these results.

Nevertheless, for a common case of the medium with absorption and multiple scattering, the problem of the derivation of $\Phi(\theta)$ is opened yet. Here, we considered the SSA and the pure scattering approach only. It is far from the real world; therefore, several next steps of the study should be executed.

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