Testing a new multiple light scattering phase function using RWMCS

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In biological suspensions the forward light scattering is done mainly by the contribution of the suspended cells. The multiple scattering is almost always unavoidable, its contribution being described either Monte Carlo simulations or by approximate analytical formula. A main challenge is to produce an analytical expression that accurately describes the multiple light scattering anisotropy. The Monte Carlo approach, embedded in the RWMCS code, moves one photon at a time and checks all scattering centers to find, at each simulation step, which one will scatter the photon. The validation of the simulation results is performed by comparing the obtained angular distribution with the predictions of the theoretical calculations reported in the literature and with the angle resolved experimental measurements performed on human red blood cells (RBCs) in suspensions at different hematocrit values. RWMCS is used further on to verify the predictions of two new effective phase function recently published. The results show a good agreement in the small RBC concentration range.

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1. Introduction

Several models to investigate the steady-state light transport in multilayered tissues have been developed so far, some of the most well-known being MCNP [1] and MCML [2]. These codes consider a package of photons moving layer by layer in a target, parts of the package being scattered at different angles, transmitted or absorbed, according with random numbers generated for each decision. In biological suspensions (like blood at different hematocrit values) light scattering is performed by the suspended cells only, and not by the bulk. In the present Monte Carlo approach, named RWMCS, the photons are moved one at a time, the simulation being essentially different as compared with the traditional Monte Carlo multilayer methods. The RWMCS code is used to test two different theoretical approached that describe light scattering anisotropy where multiple scattering is present, a typical sample being a suspension of Red Blood Cells (RBC).

2. The RWMCS code

The input parameters are the photon number, the scattering center (hereafter SC) number, the cuvette dimensions, the average scattering cross-section and volume of the SC, the anisotropy factor g and the refractive indexes of the suspension and of the glass walls of the cuvette. Before a photon is launched into the cuvette, the SCs configuration is generated using random numbers having a uniform distribution. After each photon is launched, the program checks all the SC in suspension located on the “forward” direction to determine which one is the next to interact with the photon, if any (quasi-ballistic approximation). After each scattering act, the SC counter is reset and the procedure is repeated until all the SCs are checked. Before being released form the cuvette, the roulette “spins” again to determine whether the photon is scattered back in the cuvette or is transmitted. If it is returned, the procedure is repeated until it escapes.

For each photon a record is saved containing θ, φ (the angular coordinates of the exit direction of the photon), the scattering order (the number of times the photon was scattered) and the number of reflections on the cuvette glass walls.

Moving to details, the simulation was done using a 1×1×1 mm cuvette, 10^4 photons, 90 μm^2 for the average scattering cross-section and 90 μm^3 the volume of the SC, which are typical values for a human red blood cell. The SC concentration can be expressed either in SC/mm^3, or as the hematocrit, H (the volume fraction of the SCs in suspension), or as the optical depth τ, defined as:

$$\tau = H\frac{\sigma d}{v} \qquad (1)$$

where d is the cuvette thickness, σ and v are denoting the average scattering cross-section, and the volume of the SCs (RBCs) respectively.

RBC’s light scattering anisotropy is modeled with the currently used [1-5] Henyey–Greenstein phase function:

$$f(\mu) = \frac{1}{2}\frac{1-g^2}{\left(1-2\mu g+g^2\right)^{\frac{3}{2}}} \qquad (2)$$

where $\mu = \cos(\theta)$ and $g = <\mu>$. Starting from (2) we can derive the θ probability distribution:

$$p(\theta) = \frac{1}{2}\frac{1-g^2}{\left(1-2g\cos(\theta)+g^2\right)^{\frac{3}{2}}}\sin(\theta) \quad (3)$$

A 0 value for g indicates isotropic scattering and a value near 1 indicates strong forward directed scattering. Different values from 0.95 to 0.98 were used, in agreement with [3-5]. When an interaction occurs, the value of the μ is determined by the random number ξ generated uniformly at each scattering event over the interval [0, 1], as in [1], [2], [6]:

$$\mu = \frac{1}{2g}\left[1+g^2+\left(\frac{1-g^2}{1+2g\,\xi-g}\right)^2\right] \quad (4)$$

The azimuthal angle φ is uniformly distributed over the interval [0, 2 π] and is sampled as [1], [2], [6]:

$$\varphi = 2\pi\xi \quad (5)$$

where ξ is a random number in the interval [0,1] generated using a uniform distribution.

After the deflection θ and the azimuthal angle φ are selected, the new direction of the photon in the cuvette reference frame can be calculated [1], [2], [6] using:

$$\begin{aligned}
\mu'_x &= \frac{\sin\theta\left(\mu_x\mu_z\cos\varphi-\mu_y\sin\varphi\right)}{\sqrt{1-\mu^2_z}}+\mu_x\cos\theta \\
\mu'_y &= \frac{\sin\theta\left(\mu_y\mu_z\cos\varphi+\mu_x\sin\varphi\right)}{\sqrt{1-\mu^2_z}}+\mu_y\cos\theta \quad (6)\\
\mu'_z &= -\sin\theta\cos\varphi\sqrt{1-\mu^2_z}+\mu_z\cos\theta
\end{aligned}$$

If the photon is close to the z axis than:

$$\begin{aligned}
\mu'_x &= \sin\theta\cos\varphi \\
\mu'_y &= \sin\theta\sin\varphi \quad (7)\\
\mu'_z &= sign(\mu_z)\cos\varphi
\end{aligned}$$

In (6) and (7) μ_x, μ_y, μ_z, are the direction cosines before interaction and μ'_x, μ'_y, μ'_z after the interaction.

When the photon meets the glass wall the roulette spins again to determine whether the photon escapes or is reflected back. If α_i is the the angle of incidence and α_t is the angle of transmission, they are calculated using Snell's law:

$$n_i\sin\alpha_i = n_t\sin\alpha_t \quad (8)$$

The refractive index of the medium the photon is incident from is n_{water}=1.33 and of the medium the photon is reflected on is n_{glass}=1.50. The reflexion coefficient of the light intensity is given by the Fresnel's equations [7], [8]:

$$R(\alpha_i,\alpha_t) = \frac{1}{2}\left[\frac{\sin^2(\alpha_i-\alpha_t)}{\sin^2(\alpha_i+\alpha_t)}+\frac{\tan^2(\alpha_i-\alpha_t)}{\tan^2(\alpha_i+\alpha_t)}\right] \quad (9)$$

Another random number is generated and if it is smaller than R the photon is reflected back, otherwise it escapes the cuvette.

Each photon enters the cuvette through the center of the glass wall and meets a different SC configuration, generated using random numbers. This is an alternative approach preferred to the usual modeling techniques (using a fixed SC configuration and generating photons randomly through the cuvette wall area) because it is less time consuming when accounting the margin effects. The flow chart of the RWMCS and other programming details are extensively presented in [9]. The results of the RWMCS are in good agreement with the experimental results, as presented in [10].

The main topic when solving numerically the photon transport problem is handling the multiple scattering. While for single scattering there is a good agreement in the literature [1-6], there are different models proposed to analytically describe the multiple scattering. The Monte Carlo simulation results are compared with the theoretical calculations in [4] and [12]. In [4], [11], [13], [14] the normalized photon flux is split in successive order scattering fluxes. The normalized photon flux was calculated for different SC concentration, hence optical depth. Papers [13] and [14] affirm that the normalized fluxes Φ_n corresponding to different scattering orders have a Poisson distribution with the optical depth, described by equation (10):

$$\Phi_n(\tau) = \frac{\tau^n}{n!}\cdot e^{-\tau} \quad (10)$$

The distribution of the successive orders scattering flux is presented in Fig. 1, for τ = 9.9, confirming theoretical predictions.

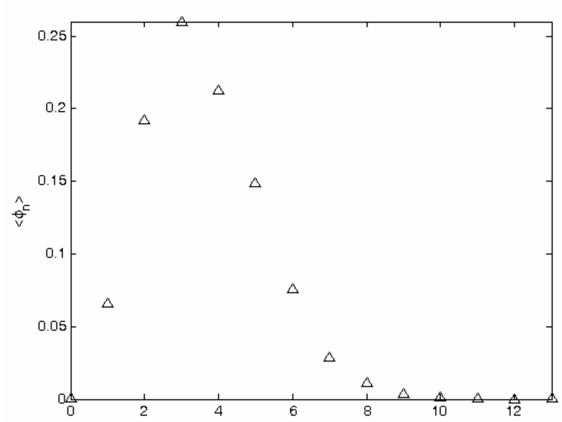

Fig. 1. The successive orders normalized scattering flux distribution for the optical depth τ = 36, corresponding to a hematocrit H = 0.036, corresponding to a RBC concentration of 4×10^5 SC/mm^3).

Fig. 2 presents the variation of the order dependent normalized flux versus optical depth. We notice again the Poisson type variation, which means a good agreement of the Monte Carlo simulations with the above mentioned models. For n = 0 the non-scattered photon flux must undergo an exponential decay, corresponding to a simple "death" model, as there is no source of photons in this scattering order. Fitting an exponential decay on the upper curve we found a very good fit, described by R^2=0.9972, very close to 1, which means the perfect fit. This match again shows a very good agreement with the theoretical calculation in [13].

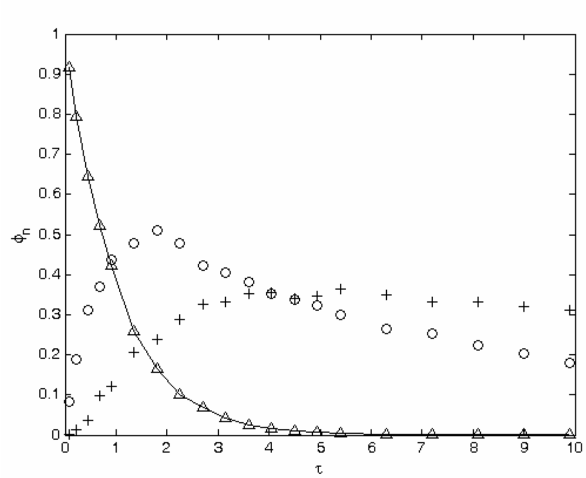

Fig. 2. The variation of the 0 order (non-scattered photons, Φ_0, triangles), first order (Φ_1, circles) and second ordered (Φ_2, crosses) normalized fluxes with the optical depth.

3. Testing the proposed phase functions

The main challenge was to find the appropriate way to describe the photon scattering anisotropy [4], [9], [11] and [13]. The Henyey-Greenstein type phase functions with a τ-dependent parameter g(τ) were introduced in order to describe the contribution of multiple scattering. Two approximated expressions have been suggested:

$$g_1(\tau) = g^{\tau} \qquad (11)$$

in [4] and:

$$g_2(\tau) = g^{G(\tau)} \quad \text{with} \quad G(\tau) = \frac{(\tau - 1)\cdot e^{\tau} + 1}{e^{\tau} - \tau - 1} \qquad (12)$$

in [11] and [13].

Figs. 3 and 4 present the variation of the normalized angular dependent flux from our Monte Carlo simulation compared with the normalized flux calculated with the single scattering and the modified Henyey-Greenstein type phase functions respectively. In the single scattering case the used value of the scattering anisotropy g was the average value of cos(θ) over the Monte Carlo simulation results. For all curves we used a target having the optical depth τ =1.35 in Fig. 3 and τ =2.25 in Fig. 4. Comparing different plots we found that the analytical function (11) ensures the best agreement with the simulation results for τ <1.8, while for τ >1.8 the best agreement is found for the function (12).

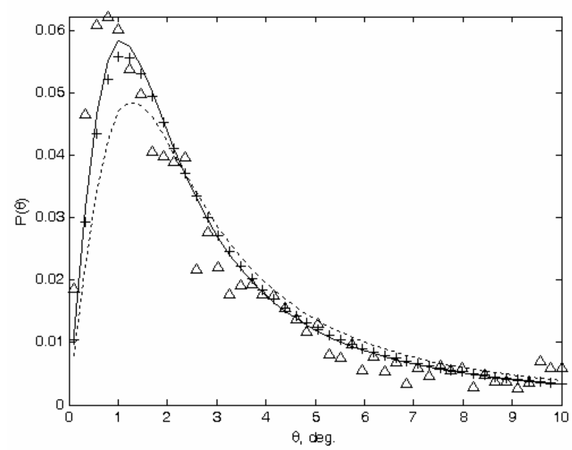

Fig. 3. The simulated normalized angular dependent flux (triangles), the normalized flux calculated with (11) (crosses), with (12) (dashed line) and the single scattering Henyey-Greenstein phase function (solid line) calculated using the average of cos(θ) for g, for a target with τ=1.35.

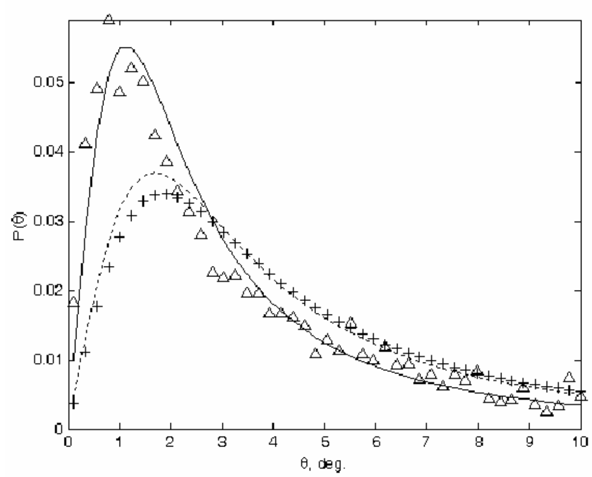

Fig. 4. The simulated normalized angular dependent flux (triangles), the normalized flux calculated with (11) (crosses), with (12) (dashed line) and the single scattering Henyey-Greenstein phase function (solid line) calculated using the average of cos(θ) for g, for a target with τ=2.25.

The anisotropy factor g has a significant variation with the optical depth. Fig. 5 presents the variation of the calculated g with the optical depth.

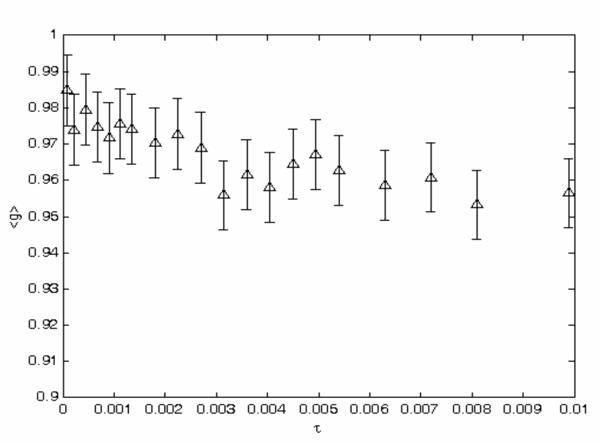

Fig. 5. The variation of the calculated g with the optical depth.

Using the RWMCS simulation we found that the anisotropy factor g_n for different scattering orders decreases with the scattering order. We also found that the parameter *g,* as calculated from our simulation, decreases as the optical depth of the target increases, which is consistent both with the predictions of the two phase functions tested with RWMCS and with the experimental results presented in [5].

4. Conclusions

The approach we used in the present paper focuses on single photon trajectory (ballistic scattering), and is essentially different as compared with the existing models that analyze statistically a photon packet at a time. The results of this simulation were compared with the theoretical predictions of the multiple scattering models [4], [12] and with experimental data [11] being in good agreement, especially in the small concentration range.

The RWMCS model, that takes into account multiple scattering and internal reflections on the cuvette walls, was used to test two new phase functions that describe multiple light scattering anisotropy on biological suspensions. We found that the analytical function (11) ensures the best agreement with the simulation results for τ <1.8, while for τ >1.8 the best agreement is found for the function (12). Both of them predict much better results that the Henyey-Greenstein single scattering phase functions, but special care must be taken when using them for targets with optical depths bigger than 3.

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