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A RANDOM WALK MONTE CARLO APPROACH TO SIMULATE MULTIPLE LIGHT SCATTERING ON BIOLOGICAL SUSPENSIONS

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Abstract The Monte Carlo approach we propose considers light scattering anisotropy, multiple scattering and internal reflection. Comparing the simulation results with the effective phase function calculations and with the experimental results on diluted RBC suspensions, we found a good agreement with the experimental data in the small concentration range.

Key words: Monte Carlo, Red Blood Cells, biological suspensions.

A Monte Carlo Simulation of Light Scattering on Suspensions

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]. The algorithm implemented in the MCML assumes that the target consists of successive layers, each one having well defined average reflection and transmission coefficients. These codes consider a package of photons to be moved layer by layer in a target, having parts of the package scattered at different angles, transmitted or absorbed, according with the random numbers generated for each decision. In biological suspensions (blood at different haematocrit values) light scattering is made by the suspended cells only, not by the bulk. In the proposed Monte Carlo approach the photons are moved one at a time, the simulation being essentially different of the traditional Monte Carlo multilayer methods.

2. THE ALGORITHM

The input parameters are the photon number, the scatter center (hereafter SC) number, the cuvette dimensions, the average cross section and volume of the SC, the anisotropy g factor and the refractive index of the suspension and of the glass wall of the cuvette. Before a photon is launched into the cuvete, the SC 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 (quasi-ballistic approximation) to interact with the photon. After the scattering act, the SC counter is reset and the procedure is repeated until all the SCs were checked. Before the photon is released form the cuvette, the roulette spins again to determine whether the it is reflected back in the cuvette or is transmitted out. If it is returned, the procedure is repeated until it escapes. The main loop is repeated until the last photon that was generated exits the cuvette. For each photon a record is saved containing the θ, φ of the direction the photon exits the cuvette, in spherical coordinates, the number of times it was scattered and the number of times it was reflected back on the cuvette glass walls.

The flow chart of the program is presented in Fig. 1.

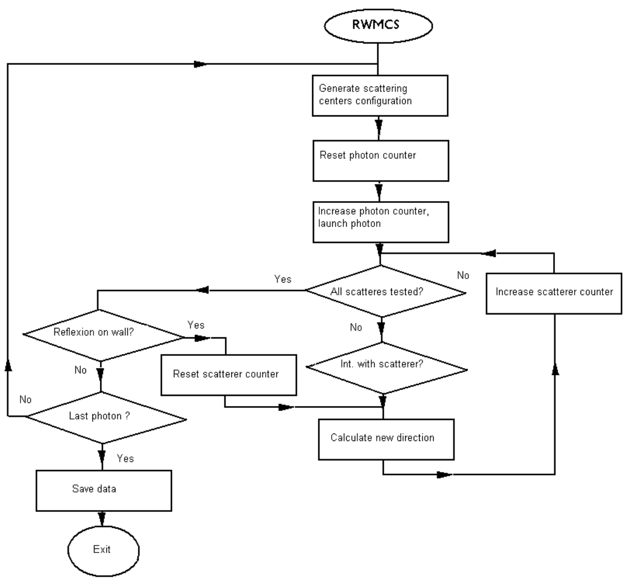

Fig. 1 – The flow chart of the program.

Moving to details, the simulation was done using a 1x1x1 mm cuvette, 10000 photons, 90 μ^2 for the effective cross section and 90 μ^3 the volume of the SC, which are typical values for red blood cells (RBC). The SC concentration can be expressed either in SC/mm^3, or as the haematocrit, H, which is the ratio of the SC volume to the total volume, or as the dimensionless parameter τ, defined as:

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

where σ is the area, d is the thickness and v the volume of the RBC.

Light scattering anisotropy for red blood cells in suspension is modeled using the Henyey – Greenstein phase function (2), which is a relatively simple expression, with one free parameter, g, currently used in light scattering simulations: [1-5]:

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

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

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

A value of 0 for g indicates isotropic scatter and a value near 1 indicates 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 spinning the roulette to obtain the new μ = cos(θ) [1], [2], [6]:

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

where ξ is a random number in the interval [0,1] generated using a uniform distribution. The azimuthal angle φ is uniformly distributed over the interval [0, 2 π] and is sampled as:

$$\varphi=2\pi\xi \tag{5}$$

After the deflection angle θ and the azimuthal angle φ are selected, the new direction of the photon in the cuvette reference frame can be calculated as in [6] using (6) and (7) where μ_x, μ_y, μ_z, are the direction cosines before interaction and μ'_x, μ'_y, μ'_z after interaction.

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

If the photon is close to the z axis than:

$$\mu'_x = \sin\theta\cos\varphi$$
$$\mu'_y = \sin\theta\sin\varphi \qquad (7)$$
$$\mu'_z = sign(\mu_z)\cos\varphi$$

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

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

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]:

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

Equation (9) is the average of the reflectances for the two orthogonal polarization directions, because after scattering on RBC of different orientations the light is no longer polarized.

When the photon meets the glass wall, the roulette spins again to determine whether the photon escapes or is reflected back. Ifα_i is the the angle of incidence and α_t is the angle of transmission, they are calculated using Snell's law. A 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 alternative is used, rather then considering the same SC configuration and generating photons randomly through the cuvette wall, because it is less time consuming for taking into account the margin effects.

3. RESULTS

Fig. 2 presents the average number of scatters a photon goes through, before exiting the cuvette. It can be noticed that beginning with $\tau = 1$ multiple scattering becomes effective. We also found that the average number of scatterings does not increase linearly with the SC concentration.

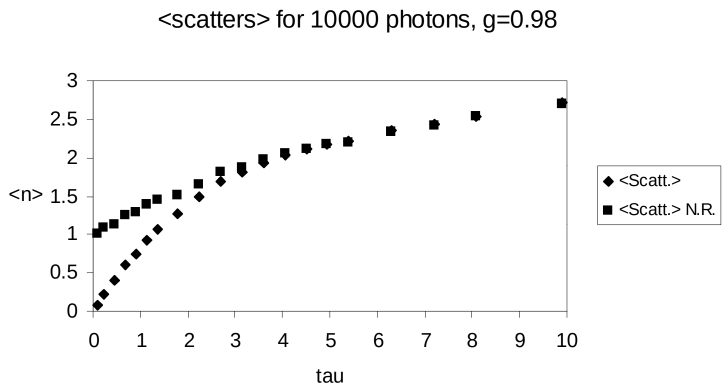

Fig. 2 - The average number of scatters versus the τ. N.R. states for average done on the photons that neither were reflected on the cuvette walls, nor escaped the cuvette without interacting.

The histogram of the number of scatters for τ=9.9, that corresponds to a haematocrit of $9.9*10^{-3}$ and therefore to concentration of 110000 SC/mm^3, is presented in Fig. 3. We notice that 33% of the photons experienced 2 interactions.

The average deflection angle θ, $<\theta>$ after experiment is presented in Fig. 4. We notice that $<\theta>$ increases with τ nonlinearly.

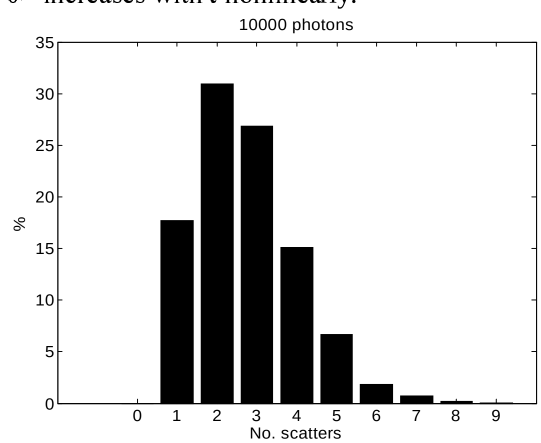

Fig. 3 - The histogram of the number of scatters for τ=9.9, H=9.9*10^{-3},110000 SC/mm^3. N.R. states for average done on the photons that neither were reflected on the cuvette walls, nor escaped the cuvette without interacting.

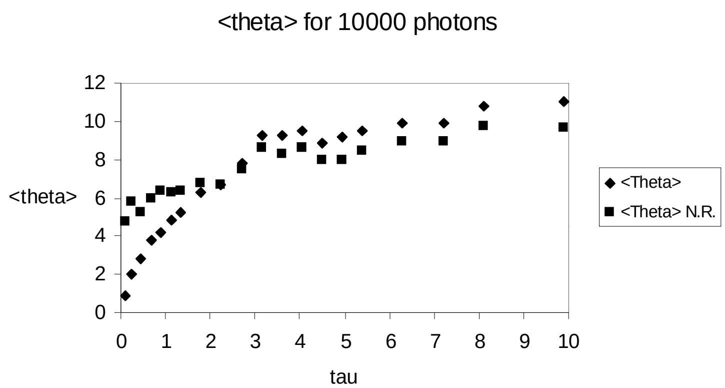

Fig. 4 - The average deflection angle θ. N.R. states for average done on photons that neither were reflected on the cuvette walls, nor escaped the cuvette without interacting.

In order to verify the output of the program we compare the results of the simulation with published results on this topic. To accomplish this task, first $\langle\cos(\theta)\rangle = \langle\mu\rangle = g$ after simulation was calculated. It is plotted versus τ and presented in Fig. 5. We notice that the effective value decreases from 0.98, the initial value down to 0.956 for H = 9.9. This result is in agreement with [5] that indicates for the anisotropy factor a value of 0.972 for physiological values of haematocrit, in a wavelength where the absorption is significant, as opposed to this paper, where it was neglected.

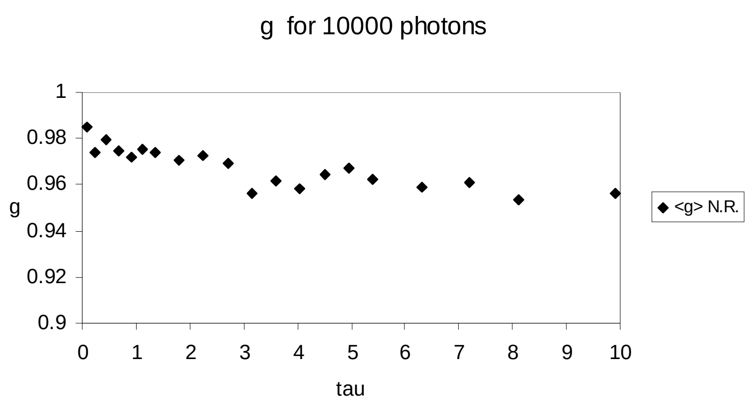

Fig. 5 - The anisotropy factor g versus τ.

In [4] and [9] the results of the theoretical calculation state that the g should be replaced with g^{τ} in the Henyey – Greenstein phase function (2). The results of this simulation agree with [4] and [9] for $\tau < 1.5$.

Another way to verify these results is to compare, at a certain deflection angle, the scattered light intensity variation with the haematocrit, with the same variation resulted from the simulation. Fig. 6 presents the experimental data and the results of the simulation for $\theta=2^o$, experimental data being taken from [10]. Again we notice a very good agreement in the small concentration range, that is $\tau < 1.5$, $H< 1.5*10^{-3}$.

4. CONCLUSIONS

The partial results of this computer simulation, using MATLAB, show a good agreement with the experimental data, in the small concentration range. Work is in progress to further improve the algorithm in the bigger concentration range, by taking into account absorption, a more accurate phase function, even if it is more time consuming and to reduce the computation time.

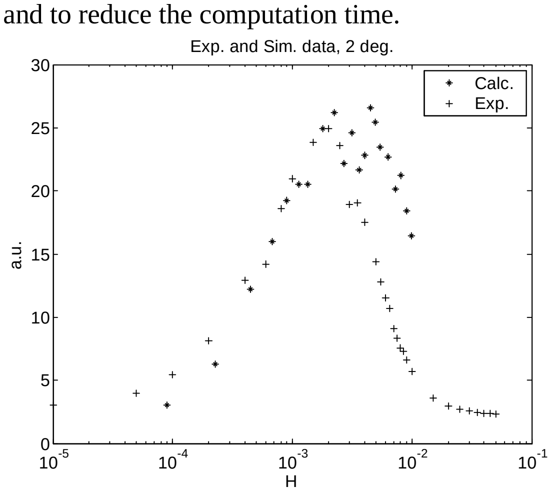

Fig. 6 - Light intensity scattered at $\theta=2^o$.

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