A fast and accurate method for the simulation of the diffusing temporal light correlation in multi-layered turbid media

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(Received 25 May 2005)

Monte Carlo simulation of the diffusing temporal light correlation in a multi-layered turbid medium is considered. A straightforward formula is introduced to calculate accurately and efficiently the autocorrelation function at any detector position. The simulation results are in an excellent agreement with an analytical solution of the correlation diffusion equation.

CLC number: O436 **Document code:** A **Article ID:** 1673-1905(2005)01-0075-03

Multiple dynamic light scattering (MDLS), which is also called diffusing-wave spectroscopy theory, can be used to investigate the dynamics of the scatters in a turbid medium[1-3]. Using a coherent laser beam to illuminate a turbid medium, a speckle pattern (an interferogram of the multiply scattered light) can be observed on the surface of the medium. Motion of the internal scatters (due to e. g. neural activities in a human brain) will result in speckle fluctuation whose rate reflects the dynamic property of the medium. Theoretically, a basic quantity in MDLS is the field temporal autocorrelation function $G_1(r_D, t) = \langle E(r_D, t') \cdot E^*(r_D, t'+t)\rangle$ (at a detection point r_D) governed by the so-called correlation diffusion equation (CDE; see Eq. (1) below)[3]. G_1 can be analytically obtained by solving the CDE for some special cases with e. g. some simple boundary conditions. Alternatively, Monte Carlo method can provide a numerical approach for getting G_1 for more general cases.

It is well known that for turbid media the Monte Carlo method is a powerful tool to simulate not only the propagation of photons[4], but also the photon correlation transportation[5,6]. In this letter, we introduce a fast and accurate numerical method to simulate the temporal correlation function diffusing in a multi-layered turbid medium. An example of 3-layered tissue medium is given for the comparison between the simulation result and an analytical solution.

In a turbid medium with the absorption coefficient μ_a and the reduced scattering coefficient μ_s', under the diffusion approximation, the scattered field autocorrelation function G_1 satisfies the following correlation diffusion equation[3]:

$$(\nabla^2 - \kappa^2(t))G_1(r,t) = -s(r) \qquad (1)$$

where $\kappa^2(t) = 3\mu_s'\mu_a + \mu_s'^2 k_o^2 \langle \Delta r^2(t)\rangle$, $\langle \Delta r^2(t)\rangle$ is the mean-squared displacement of the scattering particles in time t, k_0 is wave vector in the medium, and $s(r)$ is the source term. For a point-like source at a position r', $s(r) = s_0\delta(r-r')$.

In an N-layered medium as shown in Fig. 1, the normalized field autocorrelation function $g_1(t) = G_1(r,t)/G_1(r,0)$ for a certain photon with path α (from the source to the detector) can be calculated with the Monte Carlo method according to the following formula[5]

$$g_1^{(\alpha)}(t) = \exp\Big(-\frac{1}{3}\sum_{i=1}^{N} Y_i^{(\alpha)} k_{o(i)}^2 \langle \Delta r^2(t)\rangle_i\Big) \qquad (2)$$

where $Y_i^{(\alpha)} = \sum_{j\in \text{layer}\_i}(1-\cos\theta_{\alpha,j})$ is the dimensionless momentum transfer, the subscript j refers to the j-th scattering site along path α, $\theta_{\alpha,j}$ is the scattering angle (between the incident and scattered directions) at site j, the subscript i refers to the i-th layer, and $k_{o(i)}$ is the wave vector in the i-th layer. In our simulation, we assume the scatters undergo Brownian motions, i. e., $\langle \Delta r^2(t)\rangle_i = 6D_{B(i)}t$, $D_{B(i)}$ is the Brownian diffusion coefficient for the i-th layer.

The correlation function g_1 at the location of the detector is the weighted average of Eq. (2). Usually the following formula is used to calculate g_1[5]

$$g_1(t) = \int_0^\infty P(Y)\exp(-k_o^2\langle \Delta r^2(t)\rangle Y/3)\,\mathrm{d}Y \qquad (3)$$

where $P(Y)$ is the probability distribution of the dimensionless momentum transfer experienced by the photons arriving at the detector from the source. This distribution $P(Y)$ is numerically obtained with the Monte Carlo simulation and may fluctuate during the simulation. Note that Y varies from 0 to $+\infty$ and usually it takes a long time for the fluctuation to become small enough to satisfy a required precision. Actually, an accurate evaluation of $P(Y)$ for a large Y is not necessary since the exponential term in Eq. (3) decreases very fast when Y in-

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creases. However, in a conventional Monte Carlo implementation, which does not take the exponential term into account during the simulation, it's difficult to determine a critical value of Y, above which a low precision suffices for the convergence criterion of $P(Y)$. This degrades either the convergence speed or the accuracy in the calculation of the correlation function g_1.

In the present letter, we introduce the following formula to obtain $g_1(t)$ directly from an MCML simulation:

$$g_1(t) = \frac{1}{\sum_k w_k} \cdot \sum_k \left[w_k \cdot \exp\left(-\frac{1}{3} \sum_{i=1}^{N} Y_i^{(k)} k_{o(i)}^2 \langle \Delta r^2(t) \rangle_i \right) \right] \quad (4)$$

where the subscript k refers to the k-th photon package detected by the detector during the simulation, w_k is the remaining weight (proportional to the remaining number of photons) of the k-th photon package when it arrives the detector, $Y_i^{(k)}$ is the dimensionless momentum transfer experienced by the k-th photon package when it is in the i-th layer of the medium and can be obtained in the MCML simulation. For each photon package, the direction and length between two consecutive scattering sites are determined by the standard Monte Carlo method. During the simulation, we only need to determine straightforwardly whether $g_1(t)$ has converged (in order to terminate the simulation procedure as quickly as possible) under a required precision for $g_1(t)$.

In CDE, the thin light beam incident normally on the surface of a turbid medium is considered as a point-like source at a position $r' = (\rho = 0, z')$ (Fig. 1). For a semi-infinite medium, an explicit expression for G_1 (satisfying Eq. (1)) can be easily obtained[7,8]. While for a layered structure, one can work with a Fourier transform of G_1, obtain the solution in the Fourier space and then make the inverse Fourier transform. The analytical formula for G_1 on the surface of a multi-layered medium is[9]

$$G_1(\rho, z = 0, t) = \frac{1}{2\pi} \int \frac{f(q, z = 0, t)}{h(q, z = 0, t)} e^{-iq\rho} d^2 q \quad (5)$$

where $f(q, z=0, t)$ and $h(q, z=0, t)$ for a 3-layered medium (being semi-infinite) are given by

$$\begin{aligned} f(q, z = 0, t) &= s_0 z_0 \cdot \{\beta_1 D_1 \cosh(\beta_1(\Delta_1 - z')) \\ &\times [\beta_2 D_2 \cosh(\beta_2 \Delta_2) + \beta_3 D_3 \sinh(\beta_2 \Delta_2)] \\ &+ \beta_2 D_2 \sinh(\beta_1(\Delta_1 - z')) \cdot [\beta_3 D_3 \cosh(\beta_2 \Delta_2) \\ &+ \beta_2 D_2 \sinh(\beta_2 \Delta_2)]\} \\ h(q, z = 0, t) &= \beta_2 D_2 \cosh(\beta_2 \Delta_2)[\beta_1(D_1 \\ &+ \beta_3 D_3 z_0)\cosh(\beta_1 \Delta_1) + (\beta_3 D_3 + \beta_1^2 D_1 z_0)\sinh(\beta_1 \Delta_1)] \\ &+ \sinh(\beta_2 \Delta_2) \cdot [\beta_1(D_1 \beta_3 D_3 + \beta_2^2 D_2^2 z_0)\cosh(\beta_1 \Delta_1) + \\ &(\beta_2^2 D_2^2 + \beta_1^2 \beta_3 D_1 D_3 z_0)\sinh(\beta_1 \Delta_1)] \end{aligned} \quad (6)$$

Fig. 2 shows the normalized temporal electric-field correlation functions calculated with the present simulation method (circles) and the analytical formula (5) (solid line) for an example of 3-layered medium. From this figure one sees that the coincidence between our simulation result (obtained with the MCML method and formula (4)) and the analytical solution of the CDE is perfect (the relative error is only about 0.64%). We have done simulation for various situations of multi-layered media (including semi-infinite, 1-layer, 2-layer, 3-layer and 4-layer) and the numerical results $g_1^{(M)}(t)$ are always in an excellent agreement with $g_1^{(a)}(t)$ obtained with an analytical formula (the relative error is less than 1%). This agreement is much better than that reported in the literature since formula (4) (introduced in the present letter) for evaluating $g_1^{(M)}$ is more straightforward and accurate for implementation than the conventional formula (3). Note that the analytical formula works only for planar-stratified structures and is not reliable when the diffusion approximation is not valid (e.g., when the scattering coefficient is very small)[5], while the present method (based on the Monte Carlo method and formula (4)) always works.

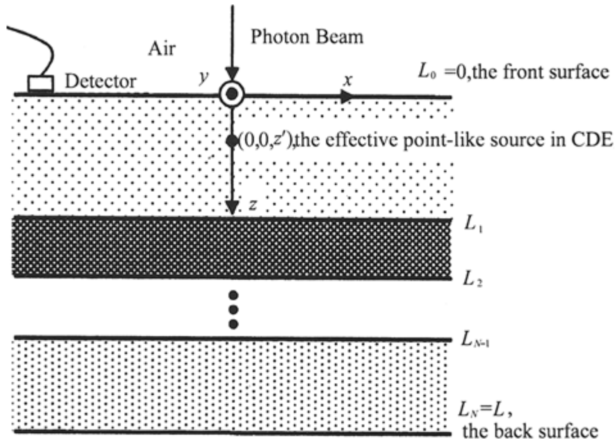

Fig. 1 A schematic diagram of the Cartesian coordinate system for a multi-layered medium. The layers are assumed to be infinite along the x-y plane

In the present letter we have studied Monte Carlo simulation of the diffusing temporal light correlation in a multi-layered turbid medium. We have introduced a straightforward formula to calculate accurately and efficiently the autocorrelation function at a detector. The simulation results for various multi-layered media are in an excellent agreement with an analytical solution of the correlation diffusion equation. To the best of our knowledge, such an excellent agreement between the Monte Carlo simulation and an analytical solution has not been reported previously.

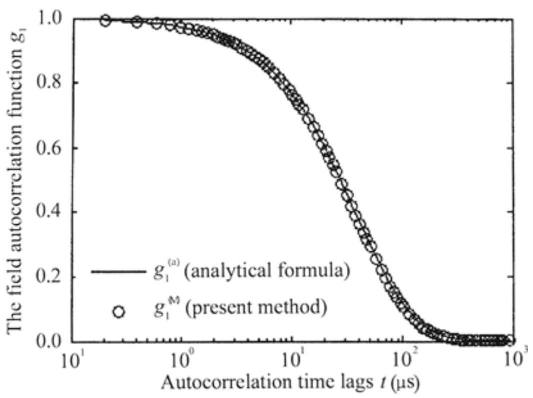

Fig. 2 The normalized temporal electric-field correlation functions calculated with the present simulation method (circles) and an analytical formula (solid line) for a 3-layered medium. The wavelength of the laser light in vacuum is $\lambda_0 = 802$ nm. The distance between the source and the detector is **$\rho = 2$ cm. The parameters for the first layer: $\Delta = 0.3$ cm, $g = 0.8$, $D_B = 1.0 \times 10^{-8}$ cm^{2}s^{-1}, $\mu_s' = 19$ cm^{-1}, $\mu_a = 0.18$ cm^{-1}, $n_r = 1.35$;**
The parameters for the second layer: $\Delta = 0.6$ cm, $g = 0.8$, $D_B = 0$, $\mu_s' = 16$ cm^{-1}, $\mu_a = 0.16$ cm^{-1}, $n_r = 1.35$;
The parameters for the third layer: $\Delta = +\infty$, $g = 0.8$, $D_B = 1.0 \times 10^{-8}$ cm^{2}s^{-1}, $\mu_s' = 22$ cm^{-1}, $\mu_a = 0.36$ cm^{-1}, $n_r = 1.35$

One of the authors (B. Luo) would like to thank H. Zhang, H. Zhu and R. Liao for their helpful discussions. This work is supported by the Science Foundation of Zhejiang Province, China (under grant number Y104255).

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