The temporal correlation transfer in layered bio-models

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Abstract. The temporal correlation functions are simulated for a two-layer model of a highly inhomogeneous medium which can be considered as the skull-brain imitation, or phantom. The temporal decay of correlations are considered for two different mechanisms of particle movement, either the Brownian diffusion, or the random velocity square mechanism. The results obtained are turned to be highly dependent on the form of the kinetics of scatterers.

1. Introduction

The temporal correlations of scattered radiation intensities in highly inhomogeneous media were firstly measured and described practically simultaneously in two famous works by Maret et al. [1] and by Pine et al. [2]. The main features of the temporal correlation transfer there has been observed: the non-analytic decay with time delay, dependence on the scattering anisotropy, and on the geometry of a medium giving rise to a number of applications. Presently the bio-medical application of the temporal correlation function turns to be one of the most important and fruitful, for determination and monitoring scatterer mobility in the tissues. The diffuse correlation spectroscopy (DCS) supplemented with the diffuse near infrared spectroscopy (DNIRS) have turned out now to be one of the most required optical tools for assessing tissue health, in regards to mammography, brain, and deep tissue injury. The diffuse photon density wave methodology, developed in mid-nineties [3, 4], consists of probing tissue with modulated near-infrared light and continues to be of great interest due to its biomedical applications [5]. In particular there was demonstrated the ability to determine the depth and degree of cutaneous and subcutaneous tissue damage critical for diabetic, venous and pressure ulcers [6, 7]. We have reported results [8] obtained within the DNIRS methodology for non-invasive measurements of reduced scattering and absorption coefficients at depths of several millimeters.

The intensity temporal correlation function presents an average of products of two random intensities observed with the time delay. The temporal decay of the field, and hence intensity correlations is determined by the kinetics of scatterers of the medium. From the beginning there was consumed that the scattering particles undergo to the Brownian diffusion. Later on there have been other kinetic mechanisms considered. Presently we perform a thorough comparison of two mechanisms within the Monte Carlo simulations. Our results produces a significant difference between these two kinds of particle mobilities, the Brownian diffusion, and the random velocity square model.

We have developed the Monte Carlo algorithm permitting to determine the blood flow parameters. For quantitative study the crucial theoretical and numerical problem to solve is a proper account for the scattering anisotropy. We perform comparative simulations of the temporal intensity correlation either with the phenomenological Heney–Greenstein (HG) phase function or the Rayleigh–Gans (RG) function, which we consider being more appropriate for the hard sphere suspension model used for
modelling a tissue; we find that for a half space geometry the results obtained for these two scattering patterns are practically coincident producing both particularly an excellent agreement with the measurement data within the frequency domain diffuse photon density wave technique; however for finite size tissue geometries results of simulations of the source-detector plot for backscattered intensity differ noticeably. We simulate the source detector plots for several sets of optical parameters, considering thus media with high, medium, and weak anisotropy, with the HG or RG patterns, and find the system with the RG pattern exhibit much stronger dependence on the anisotropy.

An application for the brain studies requires at least a two layer scull-brain model; such a model have been described earlier [9] and used for noninvasive determination of optical properties of brain within the NIRS technique. There have been admitted [10] that the optical parameters of the brain layer can be retrieved if the source-detector distance ρ exceeds some critical value, using multiple sources. In [9] the authors modelled the human head as a two layered turbid system with half-infinite lower layer, imitating the brain, for developing a non-invasive determination of optical properties of adult brain.

Recently there appeared a number of works [11, 12] on establishing a relationship of the DCS signal with blood flow. In [11, 12] the blood flow index was found fitting the multi-distant and multi-wave DNIRS measurements and simulations.

Presently we perform simulations, calculating intensity TCF, for a two-layer scull-brain model. For the brain model we use data from the known review on optical properties of tissues [13].

2. Temporal correlation decay

Let the wave equations for the field \( E \) and its Green’s function \( T \) be presented schematically as

\[
E = E_0 + T_0 \frac{\Delta \varepsilon}{4\pi} E, \quad T = T_0 + T_0 \frac{\Delta \varepsilon}{4\pi} T
\]

where subscript zero relates to a non-scattering medium, \( \Delta \varepsilon \) is the permittivity fluctuation; products mean integral convolutions. The intensity, as well as binary field correlations are the quadratic forms of the field. Since the mean of a squared random quantity is not equal to the square of the mean of the quantity, there appear correlations described with the same practically equations as the intensity itself. It brings to intensity fluctuations of order of intensity due to the field nature of the latter.

Iterating one presents the field correlation function in form of an operator series

\[
\langle \delta E^* \delta E \rangle = \langle E^* \left( T^* \frac{\Delta \varepsilon}{4\pi} + \left(T^* \frac{\Delta \varepsilon}{4\pi}\right)^2 + \cdots \right) \left(T \frac{\Delta \varepsilon}{4\pi} + \left(T \frac{\Delta \varepsilon}{4\pi}\right)^2 + \cdots \right) \rangle,
\]

where angular brackets denote statistical averaging over random permittivity inhomogeneities, and in particular over scatterer positions, \( \delta E \) is the field fluctuation.

The intensity TCF presents the 4-fold field correlator

\[
G_2(\tau) = \langle l_1 l_2 \rangle = \langle E_1^* E_1 E_2^* E_2 \rangle,
\]

Subscripts 1 and 2 determine instant observation times \( t_1 \) and \( t_2 \), with time delay, \( \tau = t_2 - t_1 \).

The Wick theorem presents the multi-fold average as a sum of pair correlators

\[
\langle \delta E_1^* \delta E_1 \delta E_2^* \delta E_2 \rangle = \langle \delta E_1^* \delta E_1 \rangle \langle \delta E_2^* \delta E_2 \rangle + \langle \delta E_1^* \delta E_2 \rangle \langle \delta E_1 \delta E_2 \rangle.
\]

The first term at the r.h.s. presents the square of intensity independent of time,

\[
l = \langle \delta E_1^* \delta E_1 \rangle = \langle E_2^* E_2 \rangle,
\]

and second term is the square of the field TCF (FTCF), dependent on time delay. One normalizes \( G_2(\tau) \), dividing it by the square of intensity, \( g_2 = G_2/G_2^2 \), producing thus the Siegert rule

\[
g_2(\tau) = 1 + |g_1(\tau)|,
\]

where \( g_1(\tau) = G_1(\tau)/G_1(0) \) is assumed being the FTCF normalized to intensity; one should to admit that \( G_1(0) \) is only part of intensity contributed by the scattered field, and does not include the
non-coherent part \( \langle E' \rangle \langle E \rangle \). As is seen the second term turns to the unit exactly at \( \tau = 0 \). Thus within the Wick’s representation, the intensity TCF appears to be a square of the binary field TCF.

In the real experiment the second term turns in (3) to be noticeably less by factor \( \beta \). In Ref. [14, the end of Section 4] this decrease of the TCF input in comparison with intensity has been discussed in details and ascribed to “number of coherence area detected”, and in particular – to the loss of polarization. In the recent work [15] it is ascribed also to the loss of coherence of the detected light. So we can consider it as a kind of an apparatus parameter, effectively diminishing the useful signal in comparison with the time independent intensity.

Describing the temporal correlation let the field be presented as a plane wave \( \exp(i k R) \) with the wave vector \( k \). The field temporal correlations exhibit due to consecutive random spatial displacements the phase lag in the oscillating factor \( \exp(i \sum_j q_j (R_j(t) - R_j(0)) \) where \( q_j \) is the scattering wave vector at the \( j \)-th scattering event. Within the Gaussian representation one obtains

\[
\langle \exp(i \sum_j q_j (R_j(t) - R_j(0)) \rangle \approx \exp(-\frac{1}{6} \sum_j \langle q^2 \rangle (\Delta R^2)).
\]

Within the Brownian diffusion law the mean quadratic displacement obeys to the linear dependence in the time delay

\[
\langle \Delta R^2 \rangle = 6D_b \tau,
\]

where \( D_b \) is the diffusion coefficient of a scatterer. Within the random velocity assumption on the mean square displacement one assumes [16]

\[
\langle \Delta R^2 \rangle = \langle V^2 \rangle \tau^2.
\]

Performed presently simulations for these two models exhibit quite different temporal behavior of temporal correlation function.

To account for the temporal decay of the TCF we multiply, in accordance with [2, Eq. (1)] the weight of a photon, which experiences \( n \) scattering events, by the factor

\[
\exp(-3^{-1}k^2 \langle \Delta R^2 \rangle \mu'_s R_n)
\]

or for Brownian diffusion –

\[
\exp(-2k^2D_b \tau \mu'_s R_n),
\]

where \( R_n \) is the random optical path, \( \mu'_s = \mu_s(1 - g) \) is the reduced scattering coefficient, \( g = \langle \cos \theta \rangle \) is the mean cosine of scattering angle \( \theta \).

One assumes also that of the sum over of scattering wave vector squares can be calculated as the product of mean values \( \sum_j \langle q_j^2 \rangle = 2nk^2(1 - g) \); numerical simulations confirm this substitution. This Bethe-Salpeter equation describes the radiation intensity transfer. However when the characteristics (temporal, spatial, frequency, angular) of the fields \( E \) and \( E' \) are different, it describes also the field correlation transfer.

3. Inverse transform for the Rayleigh-Gans pattern

The Monte Carlo method is widely used for simulation of the photon migration in tissue and tissue phantoms, mostly within the well known MCML algorithm [17]. It requires quite a large sampling volume due to the fact, that the detected photons may form very small share of the incident light. Within the MCML the signal is contributed by the photons escaping a scattering medium, thus requiring quite a large sampling due to the fact, that the detected photons may form very small share of the incident light In the modification used presently every photon contributes into the signal at every act of scattering, until it escapes the medium. In the approach presented every photon contributes into the signal; thus the number of photons can be diminished crucially also reducing the calculation time. In the standard MCML algorithm [17] only escaped photons contribute to the signal. Within our approach every scattering event contributes.

We present the scattering intensity as a sum in scattering orders (see., e.g. [18])
\[ J_\omega(\rho) = \sum_{n<n_{sc}} f^{(n)}(n)(\rho), \tag{9} \]

where \( n \)-th order term \( f^{(n)}(n)(\rho) \) is a statistical average over sampling of \( N_{ph} \) incident photons

\[ f^{(n)}(n)(\rho) = \frac{1}{N_{ph}} \sum_{i=1}^{N_{ph}} W_n^{(i)} \exp(-\mu z_n^{(i)}). \tag{10} \]

Here \( W_n^{(i)} \) and \( z_n^{(i)} \) are, respectively, the weight of the \( i \)-th photon and its distance to the boundary from the point \( r_n \) of the last scattering event, and \( R_n^{(i)} = z_1 + \sum_{j=2}^{n} r_{j-1} + z_n \) is the optical path traveled by the photon suffering \( n \) scattering events. We consider normal incidence and normal backscattering of in- and out-going pencil-like beams along cartesian coordinate \( z \) normal to the boundary \( z = 0 \).

The weight \( W_n^{(i)} \) presents a random value of integrand of multi-fold spatial integral resulting from the \( n \)-th order iteration of the Bethe-Salpeter equation. Calculating it one simulates a stochastic sequence, or trajectory, of scattering points \( r_1, \ldots, r_n \). The optical path traveled by the photon suffering \( n \) scattering events is \( R_n^{(i)} = z_1 + \sum_{j=2}^{n} r_{j-1} + z_n \). Note that Eq. (10) can be interpreted as an average of exponentials \( \exp(-\mu z_n^{(i)}) \), which describe the extinction of the radiation returning from the medium to the boundary strictly backward after the \( n \)-th act of scattering, weighted with factor \( W_n^{(i)} \).

The method is based on the well-known inverse transform procedure [19]. In particular one changes the stochastic scattering angle cosine \( \gamma_j = \cos \theta_j \), distributed with the phase indicatrix, or pattern \( p(\gamma) \) – to \( \chi_j \), uniformly distributed in interval \( 0 \leq \chi_j \leq 1 \).

\[ \chi_j = \int_{-1}^{1} p(\gamma')d\gamma'. \tag{11} \]

The HG phase function is presented as

\[ p_{HG}(\gamma) = (4\pi)^{-1}(1 - g^2)(1 + g^2 - 2g\gamma)^{-3/2}, \tag{12} \]

while the RG phase function takes the form

\[ p_{RG}(\gamma) = p(q) = (2\pi A)^{-1}4q^{-6}(\sin q - q \cos q)^2, \tag{13} \]

where \( q = kR\sqrt{2-2\gamma} \) is scattering wave vector related to the radius \( R \) of the particle, and factor \( A \) is determined with the normalization requirement, \( A = (kR)^{-2}F(2kR) \), with

\[ F(q) = 4 \int_{0}^{q} q^{-5}(\sin q' - q' \cos q')^2 dq = q^{-4}(q^4 - q^2 + q \sin 2q - \sin^2 q), \tag{14} \]

\[ 0 \leq F(q) \leq 1 \] [20].

The anisotropy of the HG phase function is determined by its parameter, mean cosine of scattering angle, \( g \), while for the RG function it determined by the product of the wave number and the radius of a scatterer, \( kR \). For given wavelength we relate parameters \( g \) and \( R \) one with another by the relation

\[ g = (4 - (kR)^{-2}\text{Cin}(4kR))/F(2kR) - 3, \tag{15} \]

where \( \text{Cin}(\chi) \) is the integral cosine [21].

We rewrite the Eq. (11) as

\[ 1 - \chi = 2\pi(kR)^{-2} \int_{0}^{q} p(q')q' dq'. \tag{16} \]

The variable \( \chi' = 1 - \chi \) can be interpreted as the cumulative probability function, which is the probability that scattering wave vector \( q' \) takes any value in the range \( q' < q \). Equation (16) is presented as \( \chi' = F(q)/F(2kR) \). The inverse transform produces readily \( q = F^{-1}(\chi) \), where
\[ x = F(2kR)x', \] with \( 0 \leq x \leq F(2kR) < 1. \]

For small \( x \), using the Lagrange inversion theorem, we find a power series of the inverse function \( q = F^{-1}(x) \),

\[
q = \frac{3\sqrt{2}}{\sqrt{2}} \left(1 + \frac{9x}{40} + \frac{2673x^2}{22400} + \frac{72063x^3}{896000} + \frac{67097232x^4}{11038720000} + \frac{282041755137x^5}{5740134400000} + \cdots \right).
\]

The indicatrix, being the derivative of cumulative function, \( F'(q) = 4(q \cos q - \sin q)^2/q^5 \), turns to zero for a sequence of points \( q_n = \tan q_n \), which with high precision can be calculated as [21]

\[
q_n = r_n - \frac{1}{r_n} - \frac{2}{3r_n^3} - \frac{13}{15r_n^5} - \frac{146}{105r_n^7} - \frac{781}{315r_n^9} - \frac{16328}{3465r_n^{11}} - \frac{6316012}{675675r_n^{13}} - \cdots,
\]

with notation \( r_n = \pi(n + 1/2), n \geq 1 \). At these points Eqs. (14) and (18) yield

\[
x_n = F(q_n) = \frac{q_n^2}{1 + q_n^2} = 1 - \frac{1}{r_n^2} - \frac{4}{3r_n^4} - \frac{31}{15r_n^6} - \frac{123}{35r_n^8} - \frac{668}{105r_n^{10}} - \frac{626152}{51975r_n^{12}} - \cdots.
\]

The values \( x_n \) are the singularity points of the inverse function \( F^{-1}(x) \).

For more accuracy, performing the numerical Monte Carlo algorithm we apply a piece-wise model \( F^{-1}(x) \) for the inverse function \( F^{-1}(x) \) in the range \( x > x_1 \). The model proposed satisfies to three requirements: continuity of \( F^{-1}(x) \), proper value, and proper singular behavior of its first derivative in points \( x_n \).

4. Simulating TCF in the scull-brain model

We study the dependence of the signal decay with the source-detector distance considering the geometry with the source and detector placed on the surface of a tissue.

We perform the simulations of the TCF within the developed algorithm, comparatively for two scattering patterns. Namely we consider a two-layer medium model, simulating a brain phantom occupying a half-space under the one-centimeter thick scull model.

Within the Brownian model the mean squared displacement (MSD) \( \langle \Delta r^2 \rangle \) depends on time delay \( \tau \) linearly, Eq. (5). Thus the \( n \)-th order term of the non-normalized field temporal correlation function for Brownian diffusion/random velocity models takes the form, respectively,

\[
j_\omega^{(n)}(\rho, \tau) = \frac{1}{N_{\text{ph}}} \Sigma_{i=1}^{N_{\text{ph}}} W_n^{(i)} \exp(-\mu_z^{(i)}) \times \left\{ \exp(-2k^2D_b\mu'_{s}R_{n}^{(i)}\tau), \exp(-3k^2(V^2)\mu'_{s}R_{n}^{(i)}\tau^2) \right\}.
\]

We perform calculations assuming the scull exhibits some dynamics with an effective diffusion coefficient ten times smaller than that of brain. Describing the model we use the averaged data from the well-known review on the optical properties of biological tissues, by S. L. Jacques [13]. Namely, considering the radiation with \( \lambda = 685 \) nm we take for the brain \( \mu'_s = 5 \) cm\(^{-1}\) and adsorption \( \mu_a = 0.0143 \) cm\(^{-1}\), while for the scull we take \( \mu'_s = 11.0 \) cm\(^{-1}\) and \( \mu_a = 0.05 \) cm\(^{-1}\); for scattering anisotropy we take \( g = 0.7725 \), and scatterer radius \( R = 250 \) nm, for brain and scull, both. For the Brown diffusion we take value \( D_b = 0.5 \times 10^{-8} \) mkm\(^2\)/s used for evaluation of the blood flow rate [12, 22]. To simplify the simulation of the multi-layered medium we neglect the refraction and reflection phenomena at the boundaries which is justified in case of small reflectivity mismatch.

In Fig. 1 we present the normalized intensity TCF \( g_\omega(\tau) \) as function of time-delay, simulated with either HG or RG phase functions, for pure brain, and scull-brain models [23]. For a half-space brain model without scull, the plots for two patterns practically coincide within the presented scale; however they turn to be noticeably different for a scull-brain models. As is seen decrease of the scattering coefficient, as well as diffusion coefficient results in decrease of the characteristic time delay, in correspondence with Eq. (20).
Figure 1. Intensity TCF $g_2(\tau)$ via time delay $\tau$ for the half-space brain model (thick solid line 0), and for the scull-brain models (1, 2, and 3), thin solid lines – RG, dash lines – HG scattering patterns; parameters of the models – in lines 0, 2a and 2b – as described above, in lines 1a and 1b – the diffusion coefficient is changed to $D_b = 10^{-8}$ cm$^2$/s, in 3a and 3b we put $\mu'_s($Scull$) = \mu'_s$; distance $\rho = 1$ cm.

However in a two-layer model the intensity as well as correlation are contributed mainly by the upper rather thick scull model at the source-detector distances of order of the characteristic length $L_{ph} = (3\mu_a\mu'_s)^{-1/2}$. To obtain meaningful knowledge on scattering properties of the brain, one is to perform measurements at larger distances. In Fig. 2 we presented the simulation results for the two-layer medium model at larger source-detector distances, $\rho = 2.5$ and 4 cm. The kinetic properties of the scull model we describe also within the Brownian diffusion picture introducing an effective diffusion coefficient, $D_{scull}$, small in comparison with the Brownian diffusion coefficient in brain. We choose two values, $D_{scull} = D_b/10$ and $D_{scull} = D_b/20$.

Figure 2. Intensity TCF $g_2(\tau)$ via time delay $\tau$. Solid line – half-space pure brain model, $\rho = 4$ cm; dash and dot-dash lines – scull-brain models: thick lines – $\rho = 2.5$ cm, thin lines – $\rho = 4$ cm; dash lines – for $D_{scull} = D_b/20$, dot-and-dash lines – for $D_{scull} = D_b/10$.

There is clearly seen that the contribution of lower layer, brain, increases with the distance increasing. Qualitatively the plots obtained demonstrate a reasonable decrease of the characteristic decay time with increase of the source-detector distance due to the fact that at larger distances the higher order scattering contribution becomes dominant. Note that therewith the absolute value of the signal diminishes strongly. As is seen with unceasing of the source-detector distances the data become close to those for a pure brain. The further increase is restrictive however with practically vanishing of the signal and the size of the human head.
In Fig. 3 we present plots for two kinetics. The difference between two models of scatterer movements turns to be significant. While decay for the random velocity model occurs in the interval from 0.1 to one ms, for the Brownian diffusion it takes a time for orders larger; comparison with measurement data indicates that the Brownian model gives more realistic evaluations for the blood flow index. There is seen also a weak but noticeable difference for the two scattering patterns; the RG phase function produces a bit faster decay as compared with the HG function.

In Fig. 4 there are presented data calculated for two source-detector separations $\rho = 2$ and 3.5 cm. As is seen from Eq. (20) for larger source-detector distances i.e. larger share of longer paths temporal correlations should decay with smaller times: the plots confirm this proposition.

5. Conclusion
The comparative analysis is performed studying the backscattering from media with the RG or HG phase functions. We have found analytic expressions for cumulative probability function in ranges of small and large values of cumulative probability. It has permitted performing simulations within the developed algorithm for the RG pattern with same effectiveness as for the HG pattern.

The scattered radiation is shown to be weakly sensitive to the form of the phase function for a medium occupying a half-space, while for a finite size scattering patterns and high scattering anisotropy it can exhibit a remarkable difference. We have pointed out the scatterers sizes for which the simple description of multiple scattering via cumulative can be realized. for a medium with larger scatterers we
find the closed approximative formula producing reliable numerical results.

Thus we find that there is a weak but noticeable dependence on the scattering anisotropy: plots for anisotropic phase function noticeably differ from that for the isotropic one for the same value of the transport length; it means that comparing calculated data and measured ones one should obtain a larger estimate for transport length with anisotropic phase function than the estimate obtained within the isotropic assumption, which is practically equivalent to the diffusion approximation; in other words the Monte Carlo simulations with anisotropic phase function for both models predict larger values for transport length than simulations within the isotropic scattering model, including the diffusion approximation predictions. We perform for the first time to our knowledge the Monte Carlo simulation of the TCF for the two-layer scull-brain model. We obtain reasonable dependence of TCF on parameters of media and geometry of measurements; the characteristic delay time increases expectedly with decreasing of the diffusion coefficient. The presence of the scull greatly increases the delay time; thus the scull effectively diminishes the share of moving scatterers. The increase of the source-detector distance decreases the delay time due to the growing dominance of higher order scattering at larger distances.

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