Bethe-Salpeter-based simulations of multiple scattering from bounded media

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Abstract. Here we present results of Monte Carlo simulations employing an effective numerical approach, based upon a description of radiative transfer in terms of the Bethe-Salpeter equation. We develop a simulation algorithm which presents a stochastic calculation of the multi-fold spatial integrals of the Bethe-Salpeter iterative solution. The algorithm is a modification of the widely known MCLM method with a signal registration recipe resulting in a significant reducing of sampling volume. For isotropic scattering the obtained results exhibit an excellent agreement with the known theoretical solution. We simulate backscattering from layers of different thickness for the Henyey-Greenstein or Rayleigh-Gans scattering patterns.

1. Generals
The radiative transfer of light continues to be of great interest mostly due to its applications in laser diagnostics of bio-tissues. The diffuse correlation spectroscopy and diffuse near infrared spectroscopy (DNIRS) are the contemporary non-invasive optical methods. For quantitative study the crucial problem to solve is a proper account for the scattering anisotropy. We perform comparative simulations of the DNIRS signals either with the Henyey-Greenstein (HG) or Rayleigh-Gans (RG) phase functions

Monte Carlo modelling, widely used simulating the optical radiation transfer in tissue and tissue phantoms, is most often performed within the well-known MCML method. In the standard MCML algorithm [1](including parallel algorithms [2]) only photons escaped the medium contribute to the signal. This method requires quite a large sampling due to the fact, that a very small share of incident photons should be detected. In the approach presented every photon contributes to the detected signal thus greatly diminishing the number of modeled photons.

The scattered radiation signal within the MCML approach is understood as a number of photons, or rays, escaping the scattering medium. We outline presently an alternative approach, based upon the Bethe Salpeter equation which differs in the way of the signal registration. Presently we perform comparative calculations within the proposed Bethe-Salpeter (BS)-based algorithm, and within the MCML-like algorithm; it turns out that the BS-based version brings to reasonable results for a sampling at least an order smaller than the standard MCML-like approach.

Let a trajectory be simulated using the conventional MCML algorithm [1]. Contributing to the detected signal, the photon packet is to escape the tissue. Thus in the conventional approach
only those trajectories containing escaped photons contribute into the signal.

Studying the transfer of optical radiation in strongly inhomogeneous media, the anisotropy of scattering is accounted for mostly within the HG phase function; it turns out being convenient due to the fact that the cumulative phase function and its inverse take closed elementary forms. Earlier we have found [3, 4] that the cumulative distribution for the RG pattern is also presented in an elementary form. We find that unlike the Mie formulas, the cumulative RG function can be presented also in an elementary form; it permits to perform the inverse transform of the

scattering is accounted for mostly within the HG phase function; it turns out being convenient due to the fact that the cumulative phase function and its inverse take closed elementary forms. We find that unlike the Mie formulas, the cumulative RG function can be presented also in an elementary form; it permits to perform the inverse transform of the angular variables.

We perform simulations of backscattering for the HG and RG patterns. We find that for backward scattering from a medium occupying a half-space highly anisotropic indicatrices result both in larger scattering intensity as compared with isotropic one in agreement with the theory, therewith the RG patterns bringing to larger values than the HG one. For thin layers, about one transport length thick, we find that the difference between two models becomes more pronounced therewith the RG patterns bringing to larger values than the HG one. For thin layers, about one transport length thick, we find that the difference between two models becomes more pronounced, for the same anisotropy.

The algorithm proposed is immediately verified comparing numerical results with the known theoretical results for isotropic scattering, in particular with the exact Milne problem solution [5, 6]; we obtain a fair agreement with this solution results.

2. The Bethe Salpeter iterative series

We describe the radiation transfer in terms of the Bethe-Salpeter equation

\[ \Gamma(\mathbf{r}_2, \mathbf{r}_1 | \mathbf{k}_f, \mathbf{k}_i) = \mu_s \delta(\mathbf{r}_2 - \mathbf{r}_1) + \mu_s \int d\mathbf{r}_3 \delta(\mathbf{k}_23) \Lambda(\mathbf{r}_2 - \mathbf{r}_3) \Gamma(\mathbf{r}_3, \mathbf{r}_1 | \mathbf{k}_23, \mathbf{k}_i), \] (1)

where \( \Gamma(\mathbf{r}_2, \mathbf{r}_1 | \mathbf{k}_f, \mathbf{k}_i) \) transforms the radiation, incident into point \( \mathbf{r}_1 \) and outgoing at \( \mathbf{r}_2 \), with initial, \( \mathbf{k}_i \), and final, \( \mathbf{k}_f \), unit wave vectors; \( \mathbf{k}_{ij} \) is the unit wave vector connecting two scattering events in \( \mathbf{r}_i \) and \( \mathbf{r}_j \), \( k_0 = 2\pi/\lambda \) is the vacuum wave number, and \( \lambda \) is the wavelength; \( p(\mathbf{k}_i, \mathbf{k}_4) \) is the normalized phase function; the single-scattering propagator \( \Lambda(r) = r^{-2}\exp(-\mu r) \) stems from the product of two complex-conjugated Green’s functions of scalar field, up to the factor \( k_0^2 \), \( \mu = \mu_s + \mu_a \) is the extinction, \( \mu_s \) is scattering, and \( \mu_a \) – adsorption coefficients.

Let \( z \) be the Cartesian coordinate, \( \mathbf{r} = (r_z, z) \), normal to the boundary of a semi-infinite medium, \( z > 0 \). Studying the angular dependence we present the outgoing field in the Fraunhofer form which describes it as the product of spherical long-range wave multiplied by the plane wave directed to the removed detection point. Then the main, non-coherent part of backscattered intensity is

\[ J(s_i, s_f) = 4\pi \int_0^\infty dz_1 \int_{z_2>0} d\mathbf{r}_2 \Gamma_\omega(\mathbf{r}_2, \mathbf{r}_1 | \mathbf{k}_f, \mathbf{k}_i) \exp(-\mu(s_f z_2 + s_i z_1)), \] (2)

where propagator \( \Gamma(\mathbf{r}_2, \mathbf{r}_1 | \mathbf{k}_f, \mathbf{k}_i) \) transforms the radiation, incident into point \( \mathbf{r}_1 \) and outgoing at \( \mathbf{r}_2 \), with initial, \( \mathbf{k}_i \), and final, \( \mathbf{k}_f \), unit wave vectors; \( \mathbf{k}_{ij} \) is the unit wave vector two scattering events in \( \mathbf{r}_i \) and \( \mathbf{r}_j \), \( k_0 = 2\pi/\lambda \) is the vacuum wave number and \( \lambda \) is the wavelength; \( \mu = \mu_s + \mu_a \) is the extinction coefficient, \( \mu_s \) is scattering, and \( \mu_a \) – adsorption coefficients; \( s_i = 1/\cos \theta_i \) \( s_f = 1/\cos \theta_f \), \( \theta_i \) is the incidence angle, and \( \theta_f \) – the angle of backscattering.

Iterating the Bethe-Salpeter equation one presents the scattering intensity as the series in scattering orders

\[ J(s_i, s_f) = \sum_{n=1}^{\infty} J^{(n)}(s_i, s_f), \] (3)

where \( J^{(n)}(s_i, s_f) \) is the n-th scattering order contribution. For isotropic scattering the lower-order terms and total intensity are exactly calculated; in particular, \( J(1,1) \approx 4.22768 \ldots \) (see [7]); for highly anisotropic scattering \( J(1,1) = 4.88970 \ldots \) [8] asymptotically.
3. The MC modeling

Within the BS-based approach we present the \( n \)-th order term \( J^{(n)}(1,s_f) \) as an average over sampling of \( N_{ph} \) incident photons

\[
J^{(n)}(1,s_f) = \frac{1}{N_{ph}} \sum_{i=1}^{N_{ph}} W_n^{(i)} p\left(\mathbf{k}_{n,n-1}^{(i)} \hat{\mathbf{k}}_f \right) \exp \left( -\mu s_f z_n^{(i)} \right),
\]

where \( W_n^{(i)} \) and \( z_n^{(i)} \) are, respectively, the weight and the distance to the boundary from the \( n \)-th scattering event point \( \mathbf{r}_n^{(i)} \).

The weight \( W_n^{(i)} \) presents a random value of the multi-fold spatial integral appeared as the \( n \)-th order iteration of the Bethe–Salpeter equation. Calculating it one simulates a stochastic sequence, or trajectory, of scattering points \( \mathbf{r}_1, \ldots, \mathbf{r}_n \).

Using the well-known algorithm of radiative transfer simulation the relative distance \( r' = |\mathbf{r}_j - \mathbf{r}_{j-1}| \) is changed to random variable \( \xi = \exp(-\mu r') \), and cosine \( t = \cos \theta \) of the scattering angle to \( \chi = 2\pi \int_{-1}^{1} p(t') dt' \); thus one transforms the 3D-spatial integral over relative coordinate \( r' = \mathbf{r}_j - \mathbf{r}_{j-1} \) in the own coordinate frame for vector \( \mathbf{r}_{j-1} \) as

\[
\int d\mathbf{r}' \Lambda_0(r') p(t) = (2\pi)^{-1} \mu^{-1} \int_0^1 d\xi \int_0^1 d\chi \int_0^{2\pi} d\phi,
\]

where \( t = t(\chi) \) is the inverse transform of function \( \chi = \chi(t) \); afterwards the integral is calculated as an average over sampling of variables \( \xi, \chi \), distributed uniformly in \([0; 1]\), and azimuth \( \phi \).

Accounting for the boundedness of the medium, one returns a photon into the medium if it reaches the boundary due to the reflection law multiplying the weight factor by the Fresnel reflection coefficient (see [9]). Thus the weight \( w_n^{(i)} \) is the product of the reflection coefficients and factor \( (\mu_s/\mu)^n \).

The calculation time depends strongly on the number of terms \( n_{sc} \) in sum (4), as well as on the sampling volume \( N_{ph} \); in [10] the number of scattering events was traced up to \( n_{sc} = 10^5 \). In figure 1 we present the simulation flowchart, describing two ways of the signal accumulation, either with Eq. (4), or with (6), for steady-state radiation, \( \omega = 0 \). For brevity we neglect the inner reflection, and adsorption.

Note that the scattering intensity calculated with (4) can be interpreted as an average of exponentials \( \exp(-\mu z_n^{(i)}) \), which describe the extinction of the photon returning from the bulk medium to the boundary after \( n \) acts of scattering. Accounting for the boundedness of the medium, one returns a photon into the medium if it reaches the boundary due to the reflection law multiplying the weight factor by the Fresnel reflection coefficient (see [9]). Thus the weight \( W_n^{(i)} \) is the product of the Fresnel reflection coefficients; in particular case of no reflection and no adsorption it is unit or zero.

To compare the present approach with the conventional one we calculate the scattering intensity alternatively, as the number of photons escaping the medium within the lines of the standard method [12, 1]. Namely we change formula (4) to

\[
J_{sc}^{(i)}(1,s_f) = \frac{1}{N_{ph}} \frac{1}{\Delta \Omega} \sum_{n=1}^{N_{ph}} W_n^{(i)} p\left(\mathbf{k}_{n,n-1}^{(i)} \hat{\mathbf{k}}_f \right) G \left( \theta_f, \theta_n^{(i)} \right),
\]

where the angular gate function \( G(\theta_f, \theta_n^{(i)}) = \Theta(\theta_n^{(i)} - \theta_f)\Theta(\theta_f + \Delta \theta - \theta_n^{(i)}) \) guarantees that the signal be detected within the solid angle interval \( \Delta \Omega = 2\pi \sin \theta_f \Delta \theta \), near the scattering angle \( \theta_f \), and \( \Theta(\theta) \) is the Heaviside step function. Thus with Eq. (6) we calculate the mean number of photons, escaping the medium after \( n \) scattering events, while within the BS-based approach we calculate the average of the Bougert-law exponentials, which appear due to the Fraunhofer approximation.
4. Backscattering within two models

The Milne problem solution as well as the lower order results known exactly permit to verify numerical simulations. It turns out that beginning with the sampling of order of $N_{ph} = 10^6$ both algorithms produce results practically coincident with the theory with an error of order of $10^{-3}$, for finite backward angles; however the BS-based one produces the reasonable results for sampling two order lower, with noticeably smaller standard deviations of order of $10^{-3}$ from the theoretical data beginning with $N_{ph} = 10^4$. In figure 2(a) there are shown angular plots of the single- and two-orders contributions calculated practically momentarily within the BS-based and MCML-like algorithms, for sampling $N_{ph} = 10^4$. We see the fair agreement of the BS-based version with the theoretical prescriptions, in contrast with the MCML-like results. It is easily understood since the data for the lower order contributions present the statistic average over $10^4$ entries for the BS-based version and over essentially smaller number of order $(10^4/N_a)$ for the MCML-like one, where $N_a$ is the number of angular intervals $[	heta; \theta + \delta \theta]$ chosen to plot the scattering intensity as function of scattering angle; we take $N_a = 30$. The similar angular plots in figure 2(b) exhibit a much better agreement between BS-based and MSML-like algorithms for $N_{ph} = 10^6$ with some advantage of the BS-based algorithm.

We presents the multiple backscattering from a half-space for the anisotropic HG or RG patterns in figure 3(a) and (b), also for two sampling volumes. The scattering anisotropy parameter $g$ (the mean cosine of the scattering angle) was taken to be $g = 0.7725$. The reasonable results for the BS-based modification is achieved beginning with the sampling $N_{ph} \sim 10^4$ while the MCML-like modification requires the sampling two order larger, $N_{ph} \sim 10^6$, to obtain the same variance level. It turns out that quantitatively the two patterns exhibit quite different angular behavior. For isotropic scattering, using BS-based algorithm and, taking $N_{ph} = 5 \times 10^7$ and $n_{sc} = 1.2 \times 10^7$ we have obtained $J(1, 1) \approx 4.225$ in an excellent agreement with the exact Milne problem solution $J(1, 1) \approx 4.228$.

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**Figure 1.** Flowchart of Monte Carlo simulation for a normal backscattering from a half-space; BS denotes the calculation based on the present approach, and MCML-like- calculation based on the count of escaped photons.
Figure 2. Backscattering intensity $J(1, 1/\cos \theta)$ from a half-space for the isotropic phase function: single scattering: • – MC simulation with algorithm (4), ○ – MC simulation with (6); sum of single- and double-scattering: ◆ – MC simulation with algorithm (4), ◆ – MC simulation with (6), solid and dots lines – analytic solutions; (a) – $N_{ph} = 10^4$, (b) – $N_{ph} = 10^6$.

Figure 3. Multiple backscattering intensity $J(1, 1/\cos \theta)$ for anisotropic, $g = 0.7725$, scattering; HG pattern: • – BS-based approach, ○ – MCML-based; RG pattern: ▲ – BS-based, △ – MCML-based; maximum scattering order – $n_{sc} = 5 \times 10^4$; $N_{ph} = 10^6$.

We study the backscattering angular dependence for the HG or RG patterns from a layer. For a half-space the anisotropic indicatrix plots both exceed the plot for isotropic scattering, in agreement with the theory. The difference between results for two patterns becomes more pronounced for the finite thickness layers. It turns out that quantitatively the two patterns exhibit quite different angular behavior. Surprisingly the angular plots change the order of magnitudes. While for the semi-infinite medium the RG plot exceeds the HG one both exceed that for isotropic scattering; their order of relative dominance becomes different for the one-transport-length thick layers. The same changes of dominance occur using the standard simulation approach.
5. Conclusion
It turns out that the widely used algorithm permits obtaining results, for specific problems, significantly faster changing the registration of the photon escape the system to the definite Bouguer-like extinction exponential describing this escape due to Fraunhofer approximation of outgoing fields.

Within the well known MCML algorithm all coordinates entering into consideration should be determined stochastically, at random. We note that within the Bethe-Salpeter based approach the final coordinate or direction is determined exactly; thus the sampling volume increases greatly.

We conclude that with increase of the anisotropy parameter $g$, the backscattering intensity increases also, for both models, in case of semi-infinite medium; however, for thin layers, of the transport length order, the HG model results in smaller scattering as compared with isotropic case, and becomes dominant relatively the RG model.

For the semi-finite geometry we conclude surely that the backward scattering for the RG model exceeds the scattering for the HG model.

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