New Approach to Solving the Radiative Transport Equation

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Abstract: We have proposed a novel method for solving the linear radiative transport equation (RTE) in a three-dimensional macroscopically homogeneous medium. The method utilizes the concept of locally rotated reference frames and can be used with an arbitrary phase function of a random medium consisting of spherically-symmetric microscopic scatterers. The angular dependence of the specific intensity written in the spatial Fourier representation is obtained as an expansion into spherical functions defined in reference frames whose z-axes coincide with the direction of the Fourier vector $\mathbf{k}$. Coefficients of this expansion are obtained by numerical diagonalization of several $\mathbf{k}$-independent tridiagonal matrices whose elements depend only on the form of the phase function. The inverse Fourier transform is then computed analytically. This results in a closed-form expression for the RTE Green's function in infinite space. Further, the plane-wave decomposition of the 3D Green's function is obtained. It is shown that the modes in this decomposition are the *evanescent plane waves*. These modes can be used to construct the solution to the boundary value problem in the slab and half-space geometries.
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Image reconstruction in optical diffusion tomography (ODT) requires formulating a mathematical model that governs propagation of near-IR light in biological tissues [1–3]. A description based on Maxwell equations is too detailed and is not currently used. A more practical option is the use of the radiative transport equation (RTE) or the diffusion equation (DE), which is an approximation to the former. Currently, the vast majority of ODT implementations rely on the DE which is much simpler mathematically. However, the diffusion approximation can not be used in many practically important cases. In particular, it is not accurate in regions with relatively low scattering or high absorption (such as, for example, voids filled with clear fluids), near sources and boundaries, and in optically thin samples. If one of the above situations is encountered, propagation of the near-IR light in tissues must be described by the RTE.

Unfortunately, the RTE is notoriously difficult to solve, even in homogeneous medium with simple boundaries. This is especially true in the case of highly forward-peaked scattering which is typically encountered in biological tissues. Numerical approaches of current importance for obtaining forward solutions to the RTE are based on the discrete ordinate method [4], including the Fokker-Planck approximation for sharply forward-peaked scattering [5], cumulant expansion [6,7], modifications of Ambarzumian's method [8,9], and different levels of the P_L approximation [10,11]. Solving the inverse problem for the RTE is an even more daunting task. Historically, the first such solution was obtained with use of Monte-Carlo simulations [12]. However, the Monte-Carlo process requires an extremely large number of random walkers to obtain statistically reliable solutions. A more commonly used alternative is the discrete-ordinate method (approximation of the angular integral in the RTE by a Riemann sum). This method was used, for example, in [13] in conjunction with an algebraic iterative technique for inverting the two-dimensional RTE. The three-dimensional inverse problem was considered in [14, 15]. A hybrid method in which the medium is assumed to be separated into highly scattering regions where the diffusion approximation is valid and non-scattering regions where ballistic (geometrical) propagation is valid was developed in [16]. This approach does not require direct solution of the RTE. A very promising emerging approach is based on the cumulant expansion [17].

An alternative to the discrete-ordinate method is the method of spherical harmonics, often referred to as the P_L approximation in cases with special symmetry. This approach has the advantage of expressing the angular dependence of the specific intensity in a basis of analytical functions rather than in the completely local basis of discrete ordinates. However, when no special symmetry is present in the problem, the method

of spherical harmonics can be carried out in practice only to very low orders. Therefore, the method of spherical harmonics has not been widely used in the context of the ODT. Recently, we have suggested a modification of the standard method of spherical harmonics [18,19]. The modification is based on expanding the angular part of each Fourier component of the specific intensity in the basis of spherical functions defined in a reference frame whose z-axis is aligned with the direction of the Fourier wave vector $\mathbf{k}$. This approach resulted in significant mathematical simplifications and was referred to as the method of *rotated reference frames* in Ref. [19].

The method is based on a generalization of ordinary spherical harmonics $Y_{lm}(\theta, \varphi)$. The latter are functions of two polar angles in a fixed (laboratory) reference frame. Equivalently, we can view them as functions of a unit vector, $\hat{\mathbf{s}}$. In this case, θ and φ are the polar angles of $\hat{\mathbf{s}}$ in the laboratory frame. More generally, both the orientation of the reference frame and the direction of $\hat{\mathbf{s}}$ can vary. Thus, we define spherical functions of a unit vector $\hat{\mathbf{s}}$ in a reference frame whose z-axis coincides with the direction of a given unit vector $\hat{\mathbf{k}}$. Obviously, there are infinitely many such reference frames. To define one uniquely, it is sufficient to consider a rotation of the laboratory frame with the following three Euler angles: $\alpha = \varphi_{\hat{\mathbf{k}}}$, $\beta = \theta_{\hat{\mathbf{k}}}$ and $\gamma = 0$, where $\theta_{\hat{\mathbf{k}}}$ and $\varphi_{\hat{\mathbf{k}}}$ are the polar angles of $\hat{\mathbf{k}}$ in the laboratory frame. We denote spherical functions of $\hat{\mathbf{s}}$ in the reference frame defined by the above transformation by $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$. They can be expressed as linear combinations of the spherical functions defined in the original (laboratory) frame according to

$$Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}') = \sum_{m'=-l}^{l} D_{m'm}^{l}(\varphi_{\hat{\mathbf{k}}}, \theta_{\hat{\mathbf{k}}}, 0) Y_{lm'}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) , \tag{1}$$

where $D_{mm'}^{l}(\alpha, \beta, \gamma)$ are the Wigner D-functions whose explicit form is given, for example, in Ref. [20].

The functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$ will used to solve the time-independent RTE

$$\hat{\mathbf{s}} \cdot \nabla I + (\mu_a + \mu_s)I = \mu_s A I + \varepsilon , \tag{2}$$

where $I = I(\mathbf{r}, \hat{\mathbf{s}})$ is the specific intensity, $\varepsilon = \varepsilon(\mathbf{r}, \hat{\mathbf{s}})$ is the source and A is the scattering operator with the integral kernel $A(\hat{\mathbf{s}}, \hat{\mathbf{s}}')$, normalized so that its integral over either variable is unity. First, we express all position-dependent functions as Fourier integrals, according to

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \int \tilde{I}(\mathbf{k}, \hat{\mathbf{s}}) \exp(i\mathbf{q} \cdot \mathbf{r}) d^3 k , \quad \varepsilon(\mathbf{r}, \hat{\mathbf{s}}) = \int \tilde{\varepsilon}(\mathbf{q}, \hat{\mathbf{s}}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k . \tag{3}$$

We then expand all angular-dependent quantities as follows:

$$\tilde{I}(\mathbf{k}, \hat{\mathbf{s}}) = \sum_{lm} F_{lm}(\mathbf{k}) Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) , \quad \tilde{\varepsilon}(\mathbf{k}, \hat{\mathbf{s}}) = \sum_{lm} E_{lm}(\mathbf{k}) Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) , \quad A(\hat{\mathbf{s}}, \hat{\mathbf{s}}') = \sum_{l,m} A_l Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) Y_{lm}^{*}(\hat{\mathbf{s}}'; \hat{\mathbf{k}}) , \quad (4)$$

where the set of coefficients $F_{lm}(\mathbf{k})$ must be found by back substitution into the original equation (2). An important feature of the proposed method is that the dependence of these coefficients on $\hat{\mathbf{k}}$ can be found analytically. It is also important to note that the expansion of $A(\hat{\mathbf{s}}, \hat{\mathbf{s}}')$ into the spherical functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$ is independent of $\hat{\mathbf{k}}$: This fact follows from the rotational invariance of the scalar product.

Substitution of these expansions into the original equation (2) results in a $\mathbf{k}$-independent generalized eigenproblem which can be algebraically reduced to diagonalization of a block-tridiagonal $\mathbf{k}$-independent infinite matrix (in practical computations, this matrix can be truncated.) It also turns out that in the case of a pointed collimated source, the first Fourier transform in (3) can be computed analytically which results in a closed-form expression for the specific intensity.

In Ref. [18], the method was applied to computing the infinite-space RTE Green's function. In Ref. [19] boundary conditions on planar interfaces have been introduced. It was shown that the developed formalism is naturally suited for solving the RTE boundary-value problem which is specified in the *half-range* of the angular variable. Ref. [19] also provides some initial numerical simulations and extensive mathematical details.

We believe that the developed method is well suited for the image reconstruction problems of ODT. The following advantages can be listed:

1. Mathematical formulation of the linearized inverse problem of the ODT requires computation of a linear integral operator which couples data to the object function (such as the near-IR absorption). When the RTE is used, the kernel of this integral operator is a product of two RTE Green's functions with an additional angular integration. If the discrete-ordinate method is used, the integration must be replaced by summation over a limited number of discrete ordinates. The method of rotated reference frames allows to perform this integration analytically. We have used this fact in Ref. [21] where the method of rotated reference frames was used to simulate data in optically thin layers.

2. In the slab and half-space geometry, the RTE Green's function is obtained as a plane-wave decomposition. Such decomposition is a required mathematical tool for application of analytical (symmetry-based) image reconstruction algorithms of Refs. [22–25]. These algorithms are independent of the diffusion approximation and were recently used for inverting the RTE with the data set of approximately 10^6 measurements [17].

3. So far, we have developed the method for macroscopically homogeneous medium. This may be insufficient for building iterative solution to the nonlinear inverse problem of the RTE. However, we have recently developed a class of nonlinear image reconstruction algorithms that utilizes only Green's functions in macroscopically homogeneous media [26]. Therefore, the method of rotated reference frames can potentially be applied to recursive solution of the nonlinear inverse problem of ODT with large data sets.

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