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Analytical solution of the simplified spherical harmonics equations in spherical turbid media

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ABSTRACT

We present for the first time an analytical solution for the simplified spherical harmonics equations (so-called SP_N equations) in the case of a steady-state isotropic point source inside a spherical homogeneous absorbing and scattering medium. The SP_N equations provide a reliable approximation to the radiative transfer equation for describing light transport inside turbid media. The SP_N equations consist of a set of coupled partial differential equations and the eigen method is used to obtain a set of decoupled equations, each resembling the heat equation in the Laplace domain. The equations are solved for the realistic partial reflection boundary conditions accounting for the difference in refractive indices between the turbid medium and its environment (air) as occurs in practical cases of interest in biomedical optics. Specifically, we provide the complete solution methodology for the SP_3, which is readily applicable to higher orders as well, and also give results for the SP_5. This computationally easy to obtain solution is investigated for different optical properties of the turbid medium. For validation, the solution is also compared to the analytical solution of the diffusion equation and to gold standard Monte Carlo simulation results. The SP_3 and SP_5 analytical solutions prove to be in good agreement with the Monte Carlo results. This work provides an additional tool for validating numerical solutions of the SP_N equations for curved geometries.

1. Introduction

Diffuse light propagation modelling in biological tissues plays an important role in biomedical optics. It finds applications in diverse areas, such as in diffuse optical tomography (DOT) imaging [1,5,15], in the characterization of biological tissues or of phantoms (synthetic tissue mimicking media) [24,25], and in light dosimetry, for instance for photodynamic therapy (PDT) [12,10]. In DOT, one seeks to image the inner optical properties of a biological tissue using boundary measurements of light emerging from the tissue following its illumination. In any case, this requires solving an inverse problem associated with the unknown tissue optical properties [11] or concentration of a fluorophore [18] or of a bioluminescent compound [17]. DOT image reconstruction algorithms heavily rely on the solution of accurate models of light propagation in turbid media. In tissue and phantom characterization, one resorts to an underlying light propagation model with homogeneous parameters and a fitting algorithm for retrieving the tissue optical parameters of geometrically simple volumes of tissue or of materials [24,25]. This resembles DOT in a way, but under much simpler and controlled settings, as DOT aims at imaging inhomogeneous tissues with generally complex boundaries. In light dosimetry, a light propagation model is resorted to for predicting the distribution of light in

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different parts of a tissue volume. Such light is used for instance in PDT to trigger an oxidative reaction by way of a photosensitizer [12,10]. All these applications obviously require accurate light propagation modelling.

The most accurate light propagation model at the meso- and macroscopic scales is recognized as the radiative transfer equation (RTE) [27,1,15] (of course at the microscopic scale Maxwell's equations are the fundamental model). The RTE is an integro-partial-differential equation for which few analytical solutions in 3D have been found for infinite or semi-infinite media, see for instance [13,21,23] and the references therein. However, for practical applications, it is burdensome to solve numerically [14], as is its high order so-called P_N approximation [4] for which also only few analytical solutions are known [22]. To deal with this complexity, one has generally resorted to the widely used diffusion equation (DE) [27]. The DE noticeably suffers from an inaccurate description of light propagation in highly absorptive tissues (vascularized tissues), low scattering (void-like tissues such as lungs), and in the case of small geometries as occurs in small animal imaging [16]. To overcome these shortcomings, the simplified spherical harmonics (SP_N) model has been proposed which is both precise under the aforementioned situations and much less computationally demanding as regards numerical solutions in comparison with the RTE and P_N [16]. For this reason, the SP_N approximation has proved to be a useful model in recent years in biomedical optics, notably in DOT [15,7,5]. The SP_N equations provide a higher order approximation to the RTE than the DE. Few analytical solutions have been developed for the SP_N equations, and in all cases, infinite or semi-infinite media have been considered [19,20,29,30]. To our knowledge, this is the first paper providing an analytical solution to the 3D-SP_N equations within a curved bounded medium. Here, we obtain such a solution for an isotropic point source located inside a spherical homogeneous medium. Specifically, we present the solution approach for the SP_3, which is readily applicable to higher orders as well, and compare the results for the SP_3 and SP_5 with those obtained with Monte Carlo simulations. We point out that analytical solutions such as that presented here, since they are exact, are very useful in validating numerical light propagation codes resorting for instance to finite differences, finite elements, or finite volumes.

A final note, the simplest way to derive the SP_N equations (so-called the formal or heuristic derivation) is to consider a planar symmetry medium [7]. One may then question the validity of the SP_N model for curved geometries such as a sphere considered here. However, deriving the SP_N equations based on the planar symmetry assumption is just one way to obtain these equations. A more rigorous approach exists based on a variational formulation, which does not require the planar symmetry assumption [26,2]. It is thus legitimate to consider the SP_N equations for any geometry.

2. The SP_N model

The SP_N equations utilize odd orders of composite moments of the radiance to approximate the RTE, since the even orders can be obtained from the odd ones [16]. It has been shown that low order SP_N equations provide sufficiently accurate results for biomedical optics [16,6]. For simplicity, we hereby consider the lowest possible order $N=3$ ($N=1$ is shown to be the DE) to both obtain applicable results and lower the complexity of the calculations presented; calculations for higher orders are similar. The SP_3 equations for the continuous-wave (CW) case are a set of coupled partial differential equations (PDEs) given by [16]

$$
\begin{aligned}
&-\nabla\cdot\left(\frac{1}{3\mu_{a1}}\nabla\varphi_1\right)+\mu_a\varphi_1=Q+\left(\frac{2}{3}\mu_a\right)\varphi_2,\\
&-\nabla\cdot\left(\frac{1}{7\mu_{a3}}\nabla\varphi_2\right)+\left(\frac{4}{9}\mu_a+\frac{5}{9}\mu_{a2}\right)\varphi_2=-\frac{2}{3}Q+\left(\frac{2}{3}\mu_a\right)\varphi_1,
\end{aligned}
\tag{1}
$$

where φ_i, μ_a, and μ_{ai} are the composite moments, zeroth, and ith-order absorption coefficients, respectively, with $i=1,2$ (note: in all that follows, it will be implicitly assumed without further repetition that index i takes on values 1 and 2); Q is the source term located inside the medium. All previous quantities generally depend on position $\mathbf{r}$, but in the present case, since the medium is homogeneous, μ_a and μ_{ai}'s are position independent.

Since we are dealing with a bounded medium, the associated boundary conditions (BCs) need to be considered. Here we use partial reflection BCs, taking into account a refractive index mismatch, since these are the most realistic for biomedical imaging. The SP_3-BC equations with the assumption of no source term on the boundary, which is the case considered here, are

$$
\begin{aligned}
&\left(\frac{1}{2}+A_1+\frac{1+B_1}{3\mu_{a1}}\mathbf{n}\cdot\nabla\right)\varphi_1=\left(\frac{1}{8}+C_1+\frac{D_1}{\mu_{a3}}\mathbf{n}\cdot\nabla\right)\varphi_2,\\
&\left(\frac{7}{24}+A_2+\frac{1+B_2}{7\mu_{a3}}\mathbf{n}\cdot\nabla\right)\varphi_2=\left(\frac{1}{8}+C_2+\frac{D_2}{\mu_{a1}}\mathbf{n}\cdot\nabla\right)\varphi_1,
\end{aligned}
\tag{2}
$$

where A_i, B_i, C_i, and D_i are constants that depend on the reflectivity function at the boundary of the medium (these constants are given in [16]).

3. Methods

Since the SP_3 equations are a set of coupled PDEs, a method for decoupling them is essential to obtain an analytical solution. This is done via eigenvalue-based diagonalization [20,29]. It should be noted that in each equation, the coupling moment (φ_2 in Eq. (1a) or φ_1 in Eq. (1b)) is added along with a coefficient. Consequently, in the homogeneous case, the SP_3 equations can be rewritten in matrix form as

$$
(\nabla^2\mathbf{I}-\mathbf{M})\mathbf{\Phi}=-\boldsymbol{\epsilon}Q,
\tag{3}
$$

with $\mathbf{I}$ being the identity matrix and

$$
\mathbf{M}=\begin{bmatrix}3\mu_{a1}\mu_a & -2\mu_{a1}\mu_a\\ \frac{-14}{3}\mu_{a3}\mu_a & \frac{28}{9}\mu_{a3}\mu a+\frac{35}{9}\mu_{a3}\mu_{a2}\end{bmatrix},\quad \mathbf{\Phi}=\begin{bmatrix}\varphi_1\\ \varphi_2\end{bmatrix},
$$