Incorporating Boundary Conditions in the Integral Form of the Radiative Transfer Equation for Transcranial Imaging

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Abstract: An integral Neumann-series implementation of the Radiative Transfer Equation that accounts for boundary conditions is proposed to simulate photon transport through tissue for transcranial optical imaging.

1. Introduction

A fundamental component to understand the underlying workings of the brain is the quantification of neurotransmitter (NT) effects. This quantification can provide insights on the communication of neuronal systems by means of synapses. Currently, neuroscientists measure these effects as membrane potential changes and the the number of action potentials using invasive methods such as craniotomy. However, *in vivo* quantification of NT actions in cerebral cortex in humans is not possible with current technologies. To overcome this issue, our research team, as part of an NIH Brain Initiative award, is developing voltage-sensitive dyes (VSDs) that can be safely used in humans to measure membrane potential changes and changes in the production of action potentials in vivo. These VSDs can be excited in the 650 nm range, and in response to changes in membrane potential, emit radiation in the near-infrared (NIR) domain.

To use the radiation emitted by the VSDs to reliably estimate the NT effects, accurate models to simulate the propagation of the NIR radiation through the brain are required. The radiative transport equation (RTE) can be used for modeling this photon propagation. We have developed an integral Neumann-series-based RTE for both homogeneous [1] and heterogeneous [2] scattering media. However an issue with this method is the implementation of the boundary conditions. When light propagates through a tissue, it suffers reflection when there is a refractive-index mismatch. This refractive index mismatch could be especially pronounced as light propagates through different tissue types in the brain, skull, and then exits the tissue to enter into the air medium. Due to the reflection occurring at these interfaces, photons are reflected back into the medium. It has been observed previously that not modeling BCs in photon transport could lead to upto 50 % or more errors in estimation of the optical coefficients of the underlying tissue [3]. Thus, to estimate the NT effects accurately, accounting for BCs in the RTE is important. The current integral version of the RTE does not account for these effects. To overcome this issue, we develop a Neumann-series-RTE version that accounts for reflection occurring when there is a refractive index mismatch. In the proposed derivation, we focus on the refractive index mismatch as light propagates from tissue to the outside medium.

2. Theory

The fundamental radiometric quantity that we will describe the RTE is the photon distribution function, a quantity that is analogous to the radiance and quantifies the density of photons at a particular location and in a particular direction. Denote the photon distribution function at location r in direction $\hat{s}$ and frequency ν by $w(r,\hat{s},\nu)$. Let the absorption and scattering coefficients at location r be denoted by $\mu_a(r)$ and $\mu_{sc}(r)$ respectively and let c_m denote the speed of light in the medium. Let $\Xi(r,\hat{s},\nu)$ denote a mono-energetic source of emission of radiation, and let $f(\hat{s},\hat{s}';r)$ denote the scattering phase function. The RTE can be written in the frequency domain as [1]

$$\hat{s}\cdot\nabla w(r,\hat{s},\nu)+\left[\mu_a+\mu_{sc}+\frac{j\nu}{c_m}\right]w(r,\hat{s},\nu)=\frac{1}{c_m}\left[\Xi(r,\hat{s},\nu)+\mu_{sc}(r)\int_{4\pi}d^2\hat{s}'f(\hat{s},\hat{s}';r)w(r,\hat{s}',\nu)\right], \quad (1)$$

where j is the imaginary unit. This equation can also be represented in an integral form in terms of a Neumann series. Let $\mathcal{X}$ and $\mathcal{K}$ denote the attenuation and scattering operators, respectively. The mathematical expression of these operators for NIR imaging have been derived previously [1,2]. In steady state, the integral form of the RTE is given by

$$w(r,\hat{s})=\mathcal{X}\Xi+\mathcal{X}\mathcal{K}w \quad (2)$$

This equation can be alternatively written in a Neumann-series form as follows:

$$w(r,\hat{s}) = \mathcal{X}\Xi + \mathcal{X}\mathcal{K}\mathcal{X}\Xi + \mathcal{X}\mathcal{K}\mathcal{X}\mathcal{K}\mathcal{X}\Xi + \dots \tag{3}$$

An intuitive way of interpreting this equation is that successive terms in this series represent successive scattering events; in fact photons that have scattered n times contribute to the term $\mathcal{X}(\mathcal{K}\mathcal{X})^n\Xi$ in this series.

To incorporate the BCs into this Neumann series, we begin with a first principles treatment of light propagation in tissue. Similar to Schweigher *et al.* [4], we define the boundary of the phantom to be an infinitesimally small thin layer just outside the phantom such that in this layer, only the reflection event occurs. This thin boundary layer is illustrated in Fig. 1a. As a consequence of the BCs, there will be reflection at the boundary. Therefore, the boundary acts as a source of photon emission given by the expression $\mathcal{R}w$. An alternative way to think about the boundary reflection is to consider it like a scattering operation, except that the scattering phase function is given by the laws of reflection. Either of these two interpretations, when modeled in Eq. (2) leads to the following form for the RTE:

$$w = \mathcal{X}\Xi + \mathcal{X}\mathcal{R}w + \mathcal{X}\mathcal{K}w. \tag{4}$$

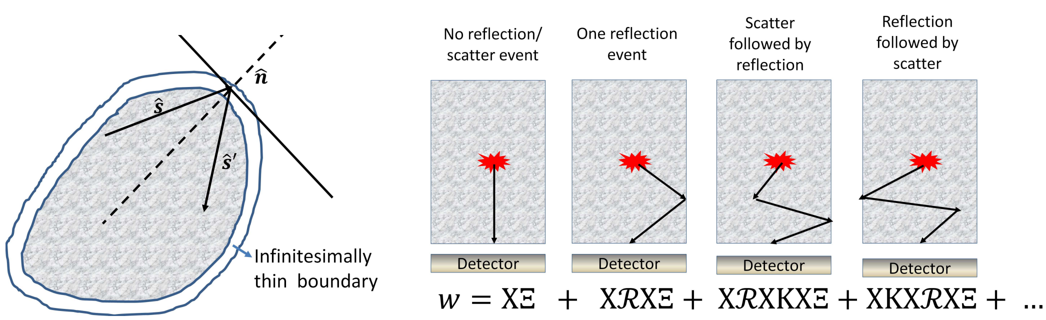
It can be shown that a formal solution of the above equation is given by the Neumann series:

$$w = [\mathcal{I} + \mathcal{X}\mathcal{R} + \mathcal{X}\mathcal{K} + \mathcal{X}\mathcal{R}\mathcal{X}\mathcal{R} + \mathcal{X}\mathcal{K}\,X\mathcal{K} + \mathcal{X}\mathcal{R}\mathcal{X}\mathcal{K} + \mathcal{X}\mathcal{K}\mathcal{X}\mathcal{B} + \dots]\mathcal{X}\Xi, \tag{5}$$

where $\mathcal{I}$ is the identity operator. A useful simplification follows if the reflection coefficient R is not very high such that $R^2 << 1$. This is typically the case with the refractive index mismatch as the photons propagate from tissue to air unless the angle of incidence is not the critical angle. As long as $R^2 << 1$, we can neglect the terms that contain the boundary kernel twice. This yields

$$\begin{aligned} w &= \mathcal{X}E + \mathcal{X}\mathcal{K}\mathcal{X}\Xi + \mathcal{X}\mathcal{R}\mathcal{X}\Xi + \mathcal{X}\mathcal{R}\mathcal{X}\mathcal{K}\mathcal{X}\Xi + \mathcal{X}\mathcal{K}\mathcal{X}\mathcal{R}\mathcal{X}\Xi + \mathcal{X}\mathcal{K}\mathcal{X}\mathcal{K}\mathcal{X}\Xi + \dots \\ &= \mathcal{X}\mathcal{R}\mathcal{X}\Xi + \mathcal{X}\mathcal{R}\mathcal{X}\mathcal{K}\mathcal{X}\Xi + \mathcal{X}\mathcal{K}\mathcal{X}\mathcal{R}\mathcal{X}\Xi + \text{Neumann series without boundary conditions.} \end{aligned} \tag{6}$$

using Eq. 3. Each of these three terms has a physical interpretation as explained in Fig. 1b.



(a) Schematic illustrating the thin boundary and reflection notations

(b) Physical interpretation of terms in the RTE that contain the boundary operator

To solve the RTE numerically, we must discretize the angular and spatial coordinates. The spatial coordinates are discretized in the voxel basis. To discretize the angular coordinates, we use the fact that the scattering kernel is only a function of the dot product of the inward and outward scattering angles. Consequently, in the spherical harmonic (SH) basis, the scattering kernel reduces to a simple diagonal form. To exploit this advantage, the RTE is solved in the SH basis. In this basis, we can derive that the Neumann series can be represented in the same form as the angular coordinates basis and is given by

$$W = \mathcal{A}\mathcal{B}\mathcal{A}\xi + \mathcal{A}\mathcal{B}\mathcal{A}\mathcal{D}\mathcal{A}\xi + \mathcal{A}\mathcal{D}\mathcal{A}\mathcal{B}\mathcal{A}\xi + \mathcal{A}\xi + \mathcal{A}\mathcal{D}\mathcal{A}\xi + \mathcal{A}\mathcal{D}\mathcal{A}\mathcal{D}\mathcal{A}\xi + \dots \tag{7}$$

where $\mathcal{D}$, $\mathcal{A}$, and $\mathcal{B}$ denote the scattering, attenuation, and boundary operators in the SH basis, respectively. The expressions for the scattering and attenuation operators in the SH basis have been derived previously [1]. We now describe the procedure to compute the expression for the boundary operator in the SH basis.

Let the normal vector to the tissue-air interface be denoted by the vector $\hat{n}$, as illustrated schematically in Fig. 1a. Then the radiance escaping along the outward direction $\hat{s}$, where $\hat{n} \cdot \hat{s} > 0$, is partly reflected at the tissue-air interface in a direction $\hat{s}'$. The direction vector $\hat{s}'$ is given by the law of reflection as

$$\hat{s}' = \hat{s} - 2\hat{n}(\hat{n} \cdot \hat{s}). \tag{8}$$

Denote the kernel that implements the BCs in the angular coordinates by $\mathcal{R}$. Using Eq. (8), we can derive that

$$[\mathcal{R}w](r, \hat{s}') = \int_{\hat{n}\cdot\hat{s}>0} R\ \delta[\hat{s}' - \hat{s} + 2(\hat{n}\cdot\hat{s})\hat{n}] w(r, \hat{s}) \mathrm{d}\Omega_{\hat{s}}, \tag{9}$$

where $\delta(\hat{s})$ is the delta function and where R is the reflectivity coefficient given by Fresnel's law. The mean refractive index is assumed to be constant within the medium, so that the boundary kernel is independent of the location r. Denote the radiance that is reflected back into the medium for the $(i, j, k)^{\text{th}}$ voxel in the SH basis by $W^r_{l',m'}(i, j, k)$. Using the definition for the SH transformation and Eq. (9), we derive that

$$W^r_{lm}(i, j, k) = R \int_{\hat{n}.\hat{s}'>0} Y^*_{lm}\{2\hat{n}(\hat{n}.\hat{s}') - \hat{s}'\} w(i, j, k, \hat{s}') \mathrm{d}\Omega'. \tag{10}$$

where $Y_{lm}(\hat{s})$ denotes the SH basis functions. Replacing $w(i, j, k, \hat{s})$ with its SH representation and further simplification yields the following expression for the elements of the boundary kernel matrix, denoted by $B_{l'm',lm}$:

$$B_{lm,l'm'} = R \int_{\hat{n}.\hat{s}'>0} Y_{l'm'}(\hat{s}') Y^*_{lm}\{2\hat{n}(\hat{n}.\hat{s}') - \hat{s}'\} \mathrm{d}\Omega'. \tag{11}$$

This expression, in conjunction with the expressions for the $\mathcal{A}$ and $\mathcal{D}$ operators, in Eq. (7), provides an analytical model to simulate photon propagation across the tissue and to the detector while accounting for BCs.

3. Implementation and validation

We have already developed and validated software to implement the Neumann-series form of the RTE in the absence of BCs for both homogeneous [1] and heterogeneous [2] scattering medium, where the latter has been implemented on NVIDIA graphics processing units to exploit the parallelizability of the execution, and has been used to model signal detectability in diffuse optical tomography [5]. We will be modifying this software to add the effect due to the terms corresponding to the BCs. We will also be validating the analytical approach by comparing to Monte-Carlo-based techniques, and evaluate the trade-offs with the analytical technique.

4. Conclusion and Future Work

An analytical approach to account for BCs in the integral form of the RTE has been proposed. The formalism shows that accounting for BCs under the assumption of low refractive index mismatch at the boundary requires adding just three terms to an already developed Neumann-series implementation that does not incorporate BCs. Current efforts are on implementing and validating the proposed formalism. A focus of ours has been on diffuse optical imaging. Meanwhile, our group is also developing photoacoustic VSDs. Thus, we are exploring the use of quantitative photoacoustic tomography (PAT) for transcranial imaging, and the use of RTE for helping to solve the optical inverse problem in PAT. The proposed formalism will help extend the usage of the Neumann-series RTE to accurately model light propagation for transcranial imaging using both diffuse optical and PAT setups.

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