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# A new Monte Carlo simulation package for light transport in biological tissues and an application to detailed analysis of the diffusion approximation accuracy near the boundaries.

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**Abstract:** We present a new Monte Carlo computational package for solving the radiative transport equation. The package is applied for numerical evaluation of the validity of the diffusion approximation for transmission and back-reflection of an incident narrowly-collimated laser beam.

**OCIS codes:** 110.6960, 290.5855, 110.5405

## 1. Introduction

Monte Carlo simulations of light propagation in tissues are widely used in biomedical optics. While some analytical or semi-analytical methods to solving the underlying radiative transport equation exist (for example, we have developed the method of rotated reference frames to that end [1–3]), Monte Carlo remains the gold standard. Many researchers write their own codes for Monte Carlo simulations but there are not so many publicly available Monte Carlo packages. One of the most frequently-used packages is MCML; it was developed by Wang, Jacques and Zheng in 1995 [4]. One of the features of this code is that it assumes illumination by a normally-incident narrowly-collimated beam onto a possibly layered slab. The problem in this case possesses cylindrical symmetry and the photon histories can be accounted for in concentric cylindrical shells. This approach improves statistics but it does not allow one to consider off-normal incidence or more general type of illumination. A more recent code by Ramella-Roman, Prahl and Jacques [5] is free of some of these limitations, and we are working along similar lines.

We are developing a new computational Monte Carlo package that is intended to be applicable to many problems that arise in biomedical imaging. The scalar version of the code is currently freely available at <https://www.cbica.upenn.edu/vmarkel/CODES/index.html> and the vector version (which accounts for polarization of light) is under development and will be made available in the future. The code is developed in modern Fortran language with extensive use of vectorization of all computationally-intensive operations. We allow arbitrary incidence on a rectangular sample, including collimated or isotropic surface or internal sources and a variety of phase functions. Statistics can be accumulated either inside the volume or at the surface and the specification of the region where the statistics is accumulated is flexible and in general different from the spatial region occupied by the sample. No symmetry is assumed. The codes can compute either the density of energy or the current of energy (a vector) or the specific intensity directly, either at fixed angles or in a range of angles, or a combination of the above quantities. The use of vectorization allows us to increase the code efficiency to a point at which simulation of rather extreme cases becomes possible. For example, we show below a simulation for a slab filled with a highly scattering medium characterized by the scattering-to-absorption coefficient ratio  $\mu_s/\mu_a = 500/0.03$ , highly forward peaked forward scattering with the scattering asymmetry parameter  $g = 0.98$  and the slab width  $L_z = 100\ell^*$ , where  $\ell^* = 1/[\mu_a + (1-g)\mu_s]$  is the transport mean free path. Although we do see strong statistical fluctuations in this case, Monte Carlo simulations at such large optical depth and highly forward-peaked scattering are very challenging.

## 2. Investigation of the diffusion approximation

The diffusion approximation is very important in optical tomography. While the conditions of validity of the diffusion approximation are well understood when the source and the point of observation are far from the boundaries, the situation is not so simple if the above condition does not hold. Derivation of the correct boundary conditions for the

diffusion equation [6] was an important step towards practical applicability of diffuse optical tomography. However, the boundary conditions for the diffusion equation are in principle different from the half-range boundary conditions of the radiative transport equation. Therefore, the specific intensity computed by the diffusion approximation can not possibly be correct near the boundaries. However, it can be approximately correct for directions of propagation that are of interest, i.e., towards the detector. The problem is mathematically related to the existence of boundary layers near the diffuse-nondiffuse interfaces. An interesting observation is that the boundary layers always exist independently of the size or width of the sample. However, as we will see in the preliminary results below, some signatures of the transmitted intensity (computed right at the boundary) become more diffuse when the width of the sample is increased.

Another important consideration is that the diffusion approximation itself can be formulated in more than one way [7]. The variations concern the definition of the diffusion coefficient and the shape of the source. Here it is appropriate to recall that the source of the transport equation is a function of position and direction while the source of the diffusion equation is a function of position only. The anisotropy that can be present even in spherically-shaped transport source is then mimicked by a deviation from the spherical symmetry of the diffuse source (sometimes this is referred to as the formation of a dipole). In general, however, there is no unique prescription for defining the diffuse source and the problem becomes more severe near the boundaries.

The applicability of the diffusion approximation was in fact investigated rather vigorously about 30 years ago (see for instance Ref. [8]) and the general tendencies are clear. The diffusion approximation becomes more accurate when the scattering is increased relative to the absorption and when the distance between the source and the point of observation is increased. However, we believe that, given a number of outstanding questions such as the question of correct choice of the diffuse source function [7] and the influence of the boundaries, this old problem can benefit from a fresh and more detailed look, especially with the aid of more powerful computational tools that are currently available.

### 3. Preliminary numerical results

Irrespective of the source, the diffusion approximation predicts that the density of electromagnetic energy and the normal component of the energy current are the same functions at the medium surface modulo multiplication by a constant. Here the density is defined by  $u(\mathbf{r}) = \int I(\mathbf{r}, \hat{\mathbf{s}}) d^2s$ , the current is  $\mathbf{J} = \int \hat{\mathbf{s}} I(\mathbf{r}, \hat{\mathbf{s}}) d^2s$ , and  $I(\mathbf{r}, \hat{\mathbf{s}})$  is the specific intensity at the point of observation  $\mathbf{r}$  and in the direction of the unit vector  $\hat{\mathbf{s}}$ . Indeed, recall that one of the equations that make up the diffusion approximation is the Fick's law,  $\mathbf{J}(\mathbf{r}) = -D\nabla u(\mathbf{r})$ . On the other hand, the most general boundary condition of the diffusion equation is  $u(\mathbf{r}) + \ell \hat{\mathbf{n}} \cdot \nabla u(\mathbf{r}) = 0$  where  $\mathbf{r} \in \partial V$  is at the surface of the volume occupied by the sample,  $V$ , and  $\hat{\mathbf{n}}$  is the outward unit normal at the point  $\mathbf{r}$  (the surface is assumed to be regular). Combining these two equations, we obtain  $u(\mathbf{r}) = \ell D \hat{\mathbf{n}} \cdot \mathbf{J}(\mathbf{r})$  for  $\mathbf{r} \in \partial V$ . The constant  $\ell$  is the extrapolation distance [6] that characterizes the boundary. If the above linear proportionality does not hold, the diffusion approximation can not be accurate.

In Fig. 1, we illustrate the above relation in the transmission measurements for slabs of various thickness. We have chosen the parameters of the medium to be close to the typical values of biological soft tissues, i.e.,  $\mu_s/\mu_a = 500/0.03$  and the scattering asymmetry parameter  $g = 0.98$ . The optical depth of the sample varied from  $L_z = 2\ell^*$  to  $L_z = 100\ell^*$ . It can be seen that, for sufficiently thick samples, the proportionality indeed holds.

However, to make sure that the diffusion approximation is indeed accurate in all these cases, one also needs to demonstrate that the angular dependence of the radiation exiting the medium is accurately described by the diffusion approximation. In diffusion theory this dependence is described by the simple cosine function of the angle with respect to the normal; this dependence is independent of the position on the surface. In reality, the angular dependence of the specific intensity is different at different points on the surface. This is illustrated in Fig. 2. Here we compare the lateral and the normal components of the energy current at different points at the surface. The lateral current is always directed away from the axis of the source (as one could expect on physical grounds). However, this effect can not be captured by the diffusion approximation. In very optically thick slabs, however, the notion of the incident axis becomes not so important as the light propagating over a large optical depth “forgets” about the position of the source. In this case, the lateral components of the current approach zero. However, this is compatible with any cylindrically-symmetric function, not just with the  $\cos\theta$  dependence that is characteristic of the diffusion approximation. Therefore, more detailed investigation of the dependence  $I(\hat{\mathbf{s}})$  is required to make a more quantitative conclusion about the accuracy of the diffusion approximation.

We finally note that the simulation for the optical depth  $L_z = 100\ell^*$  is very challenging and required on the order of  $10^{11}$  photons. Only a small fraction of these photons was absorbed. The rest exited through the slab surfaces.

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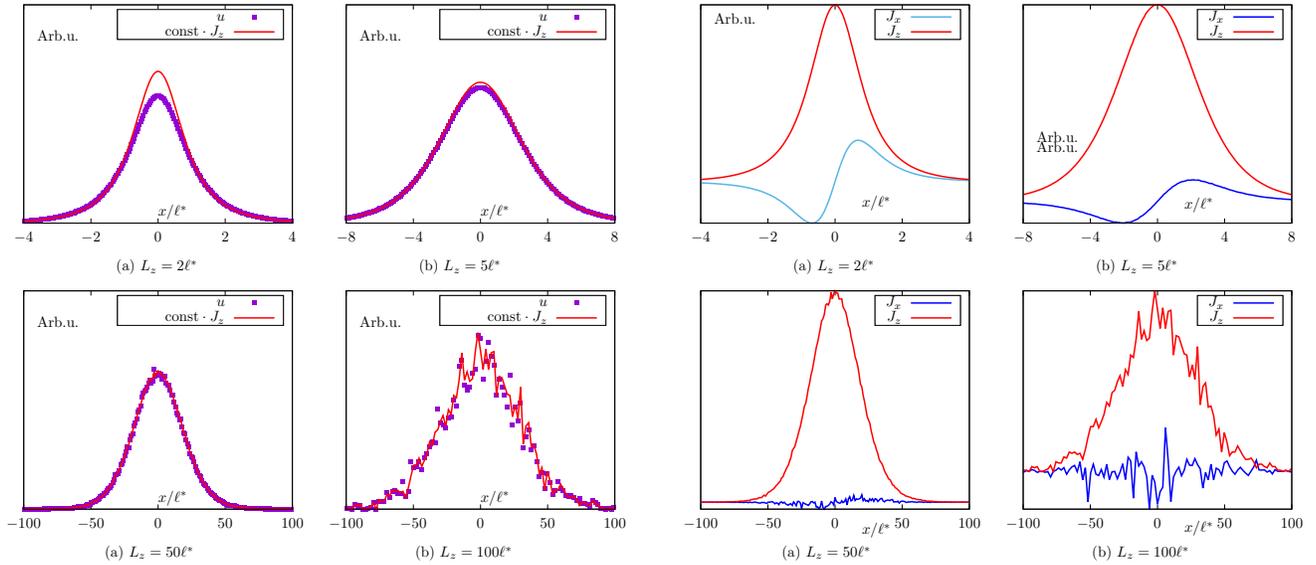


Fig. 1. (left) Comparison of the energy density  $u(x)$  and the normal component of the energy current  $J_z(x)$  at the exit surface of a slab of the width  $J_z$ . The  $X$ -axis is parallel to the surface of the slab and intersects with the axis of the incident beam at the point  $x = 0$ . The empirically found constant is  $\text{const} = 1.7$ . The two functions can be made to coincide with good precision (modulo the correct choice of  $\text{const}$ ) in the cases  $L_z = 50\ell^*$  and  $L_z = 100\ell^*$  but not in the cases  $L_z = 5\ell^*$  and  $L_z = 2\ell^*$ .

Fig. 2. (right) Comparison of the normal and lateral energy current components  $J_z(x)$  and  $J_x(x)$  in the same geometry as in Fig. 1. The component  $J_x(x)$  can not be correctly predicted by the diffusion approximation except in the limit when it is zero. Large deviations of  $J_x$  from zero in the case  $L_z = 100\ell^*$  are insignificant and can be explained by statistical fluctuations due to an insufficient number of photons used (the case  $L_z = 100\ell^*$  with the optical parameters used here is extremely challenging for Monte Carlo simulations).

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