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Relation between fluence rate and mean photons pathlengths: an alternative option for Monte Carlo-based calculations of fluence

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ABSTRACT

Usually, in biomedical optics, the average photon fluence rate, evaluated in a subvolume of a propagating medium, is obtained by Monte Carlo simulations by calculating the power deposited by photons absorbed in the subvolume. We propose an alternative method based on evaluating the average path length traveled by all photons injected within the subvolume. Application examples are given. This method also works for a zero absorption coefficient and for a nonconstant spatial distribution of the absorption coefficient within the subvolume. The proposed approach is a re-visitation of a well-known method applied to nuclear and radiation physics. The results obtained show that a potential advantage of the proposed method is that it can improve the convergence of Monte Carlo simulations. Indeed, when calculating the fluence in a region of interest with the proposed method, all photons passing through the region are considered. Whereas with the traditional approach, only "absorbed" photons are considered. In the latter case, this can produce a poorer Monte Carlo statistic for the same number of photons launched.

Keywords: Fluence Rate, Monte Carlo simulations, Mean photons pathlength

1. INTRODUCTION

The photons fluence rate is a fundamental quantity for describing the interaction of light with biological tissues when applications of biomedical optics are considered.[1–5]

Until nowadays, the modeling of photon fluence rate $\Phi(\vec{r})$ with Monte Carlo (MC) simulations in biomedical optics has mainly been performed with the method originally conceived by Wang *et al.*[6] and largely applied since many years.[7–12] The method uses and exploits the determination of the fraction of absorbed light power in a small tissue volume. However, $\Phi(\vec{r})$ can be assessed by other available methods. For this reason, and considering the importance of $\Phi(\vec{r})$ in many applications, we propose here an alternative approach based on photons pathlengths instead on the absorbed power.

With this purpose, in the present contribution we will exploit a method currently utilized in nuclear physics[13–17] but, to the best of our knowledge, never adopted in biomedical optics. Indeed, it is true that there is a tight link between $\Phi(\vec{r})$ and the length of the random paths[18] traveled by all the emitted photons in the considered medium.[19] This method can also be applied as an alternative approach to assess $\Phi(\vec{r})$ in MC simulations. For the sake of completeness, the classical method will also be used to assess $\Phi(\vec{r})$ in MC simulations. For simplicity we will call the pathlength based method, PBM, and the "classical" absorption based method, ABM.

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2. THEORY

Let's consider a medium of volume V with absorption coefficient[5] $\mu_a(\vec{r})$ and scattering coefficient[5] $\mu_s(\vec{r})$ with $\vec{r} \in V$ and external surface Σ. The medium is illuminated by both internal and external light sources emitting a total power $\mathcal{P}_e$. Let also be a subvolume $V_i \subseteq V$.

2.1 Calculation of the average fluence in a sub volume with the Absorption Based Method (ABM)

According to the classical theory (utilized in MC simulations), when $\mu_a(\vec{r})$ is constant over V_i, the average fluence inside V_i can be calculated as[6]

$$\langle \Phi_i \rangle_{\mathcal{P}_{A_i}} \equiv \langle \Phi_i(\mu_{a_i}) \rangle = \frac{\mathcal{P}_{A_i}}{\mu_{a_i} V_i}, \tag{1}$$

where $\mathcal{P}_{A_i}$ is the absorbed power inside V_i and where the subscript $\mathcal{P}_{A_i}$ is used to remember that $\langle \Phi_i \rangle$ is computed by using the absorbed power $\mathcal{P}_{A_i}$, i.e., it pertains to ABM. Equation (1) represents the classical model, where $\mathcal{P}_{A_i}$ is estimated by assessing the fraction of absorbed light power in V_i.

2.2 Calculation of the average fluence in a sub volume with the Pathlength Based Method (PBM)

Within the scheme of the radiative transfer it possible to show that the average fluence inside V_i can be calculated as[19,20]

$$\langle \Phi_i \rangle_{\langle \ell_i \rangle} \equiv \langle \Phi_i \rangle = \frac{\mathcal{P}_e}{V_i} \langle \ell_i \rangle, \tag{2}$$

where $\langle \ell_i \rangle$ is the mean pathlength traveled by all emitted photons inside V_i, $\mathcal{P}_e$ is the total power of the internal and external light sources illuminating the medium. We notice that the subscript $\langle \ell_i \rangle$ is to remember that $\langle \Phi_i \rangle$ is computed by using the mean pathlength $\langle \ell_i \rangle$, i.e., PBM. This relation establishes a straightforward connection between average fluence inside a subvolume and average pathlength spent by all emitted photons inside the same subvolume and it is valid in all generality within the steady state RTE.[19]

Thus, there are available two independent relations that can be used to calculate the average photon fluence rate inside a sub volume V_i of a medium. These two relations can be exploited inside MC simulations to perform a calculation of the CW fluence distribution inside any medium that can be described by absorption and scattering properties. In the next section these two kinds of calculation will be exploited and the obtained results synthetically shown.

3. RESULTS

In section by using MC simulations it is calculated the mean fluence rate with the ABM and the PBM. The aim of this computational exercise is to allow us to highlight some peculiarities related to the numerical convergence of these two types of calculation.

We consider the case of a 100-layered laterally infinite slab. For this purpose, let we start with a laterally finite 100-layered slab of 10 mm total thickness having top surface S and composed by 100 layers of single thickness $L = 0.1$ mm and volume $V_i = SL$ each. We have considered all the layers with the same optical parameters μ_a, μ_s, refractive index $n = 1.4$ and anisotropic scattering phase function described by an Henyey-Greenstain model with asymmetry factor $g = 0.8$.

The external medium has refractive index fixed to $n_{out} = 1$. An external plane wave of unitary photon flux is considered normally impinging to the slab top surface (i.e., an impinging flux vector of intensity $I_e = \frac{\mathcal{P}_e}{S} = 1$ mW mm^{-2}, for more details see Refs. 21,22). This is equivalent to have $\mathcal{P}_e/S = 1$ mW mm^{-2} (constant ratio even when S goes to infinity as in the case of a laterally infinite extended slab). Thus, for the selected light source and layered slab geometry we can rewrite Eq. (2) for any given layer of the slab "i" ($i = 1, 2, \ldots 100$) as:

$$\langle \Phi_i \rangle_{\langle \ell_i \rangle} = \frac{\mathcal{P}_e}{SL} \langle \ell_i \rangle = I_e \frac{\langle \ell_i \rangle}{L} \qquad (\mathrm{Wmm}^{-2}), \tag{3}$$

where $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$ and $\langle \ell_i \rangle$ are the average fluence and pathlength, respectively, in the layer "i". We note that both equalities in Eq. (3) hold for a finite slab, while we must use the second equality for a laterally infinite slab as in the present case. It is worth to note that in a laterally infinite slab the average pathlength $\langle \ell_i \rangle$ traveled in a layer "i" is independent of the choice of a point source in the plane wave. This property can be exploited to simplify the MC simulations where we can thus choose a single point as source. In the implementation of the MC method we used the Albedo-rejection method[5,19,23,24] and for each injected photon was kept track of the pathlength and the number of photons absorbed in each layer, which were used for the calculation of $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$ [Eq. (2)] and $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$ [Eq. (1)], respectively. Therefore, each MC simulation was used for the calculation of $\langle \Phi \rangle$ in each layer according to ABM and PBM. This allows to compare the convergence features of the two methods. We used a combination of the optical properties where $\mu_a \in \{10^{-6}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$ mm^{-1} and $\mu_s \in \{0,\ 0.1,\ 1\}$ mm^{-1} (i.e., 18 combinations of optical properties). For each combination we run 100 independent MC simulations with 10^6 injected photons per simulation for a total of 10^8 injected photons. Since the ABM and PBM methods were implemented within the same structure of each simulation, the calculations with ABM and PBM were also carried out for the same total number of photons packets N *and*, they also had the same computation time. This fact guarantees that the comparisons of their results give a significant information on convergence of the two methods.

In Fig. 1 we have shown $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$ as a function of $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$. As it can be expected, we observe a linear

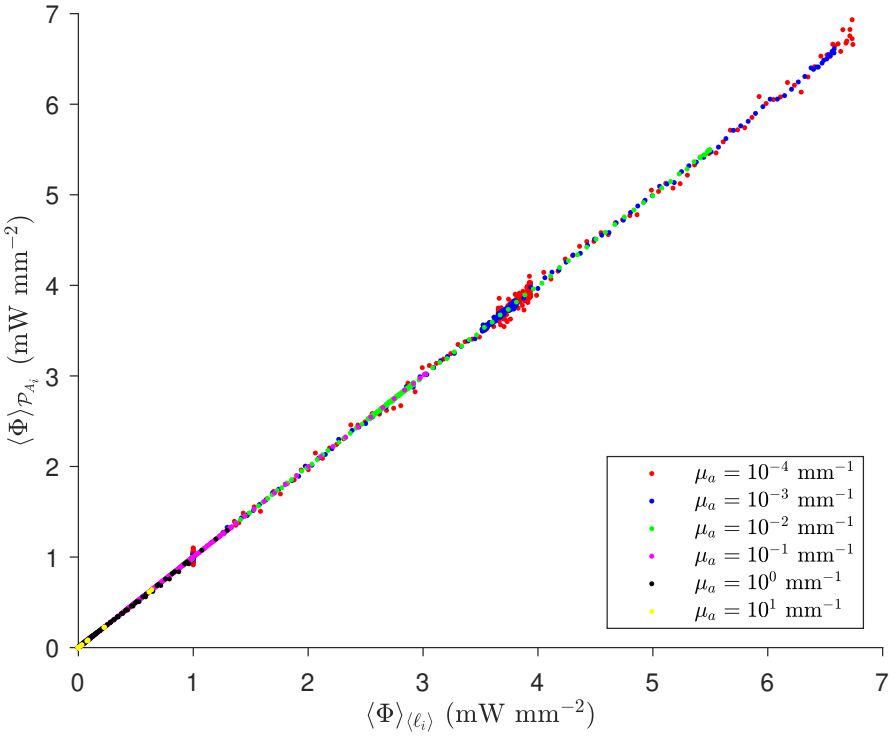

Figure 1. Mean fluence values, computed with the PBM [$\langle \Phi_i \rangle_{\langle \ell_i \rangle}$] and ABM [$\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$] methods, for each of the 100 layers and 18 different combinations of μ_a and μ_s (see text) for a total of 1800 points ordered by the increasing values of the fluence.

relationship, where the observed random distance from the identity line is due to the statistical intrinsic noise in the MC method.

The consistency between ABM and PBM can be verified by defining and calculating

$$R_i = \frac{\langle \Phi_i \rangle_{\mathcal{P}_{A_i}} - \langle \Phi_i \rangle_{\langle \ell_i \rangle}}{\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}}, \tag{4}$$

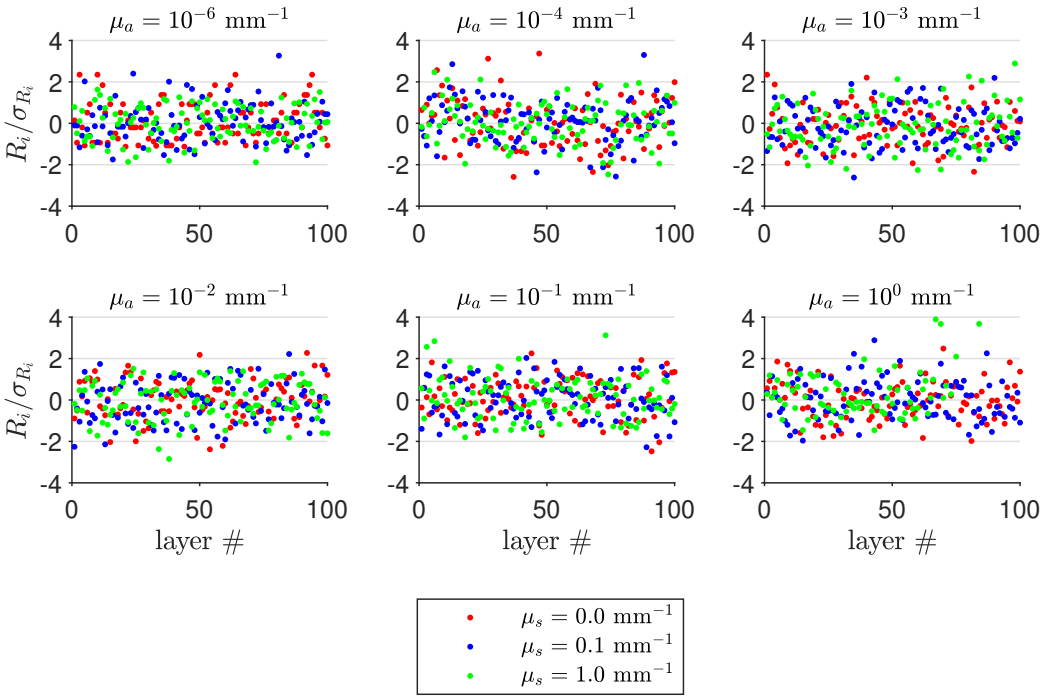

Figure 2. Consistency of the $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$ and $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$ MC data as a function of the layer number # (see text). The range for the abscissa (ordinate) axis is the same for all the panels.

i.e., the discrepancy between $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$ and $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$ normalized to the latter. If the MC values are statistically consistent, the parameter R_i must be $\lesssim 3\sigma_{R_i}$ (99.9 percentile), where σ_{R_i} is the standard error of the mean of R_i. Thus in Fig. 2 we show for the case here analyzed R_i/σ_{R_i} as a function of the layer number #. Figure 2 clearly shows that the deviations between the two calculated values are usually within two standard errors and this proves the consistency of the two calculations.

However, from Fig. 1 it is not possible to decide if the distance of the data from the identity line is mainly due to a statistical variability of the ABM or PBM or both. Further, no information appears on the role of different μ_s values. To clarify this point in Fig. 3 we have shown the relative error on the fluence, $RE_{\langle \ell_i \rangle}$, for the PBM method, i.e.,

$$RE_{\langle \ell_i \rangle} = \frac{\sigma_{\langle \Phi_i \rangle_{\langle \ell_i \rangle}}}{\langle \Phi_i \rangle_{\langle \ell_i \rangle}}, \tag{5}$$

where $\sigma_{\langle \Phi_i \rangle_{\langle \ell_i \rangle}}$ is the standard error of the mean of $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$; and the relative error on the fluence, $RE_{\mathcal{P}_{A_i}}$, for the ABM method, i.e.,

$$RE_{\mathcal{P}_{A_i}} = \frac{\sigma_{\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}}}{\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}}, \tag{6}$$

where $\sigma_{\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}}$ is the standard error of the mean of $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$. Figure 3 clearly indicates that the ABM has the tendency to generate larger relative errors compared to the PBM. By increasing μ_a the errors of ABM and PBM become similar. For values of absorption around $\mu_a = 10^{-2}$ mm^{-1}, typical, e.g., in Near Infrared Spectroscopy (NIRS), the relative error for ABM is still ∼1-2 orders larger than that for PBM. Because the two methods are applied to the same simulation (i.e., for the same number of injected photons $N = 10^8$, and the same computation time), the results provide an unambiguous information of the faster convergence of the PBM method.

It is important to notice that the relative error of a simulated quantity characterizes the reliability of the simulated value.[25] Therefore, in the comparison between ABM method and PBM method this choice is motivated by the fact that in this way we characterize the reliability of the simulated data. In general, a MC result should show a relative error lower than 0.1 to produce reliable confidence intervals of the simulated data.[25] About the

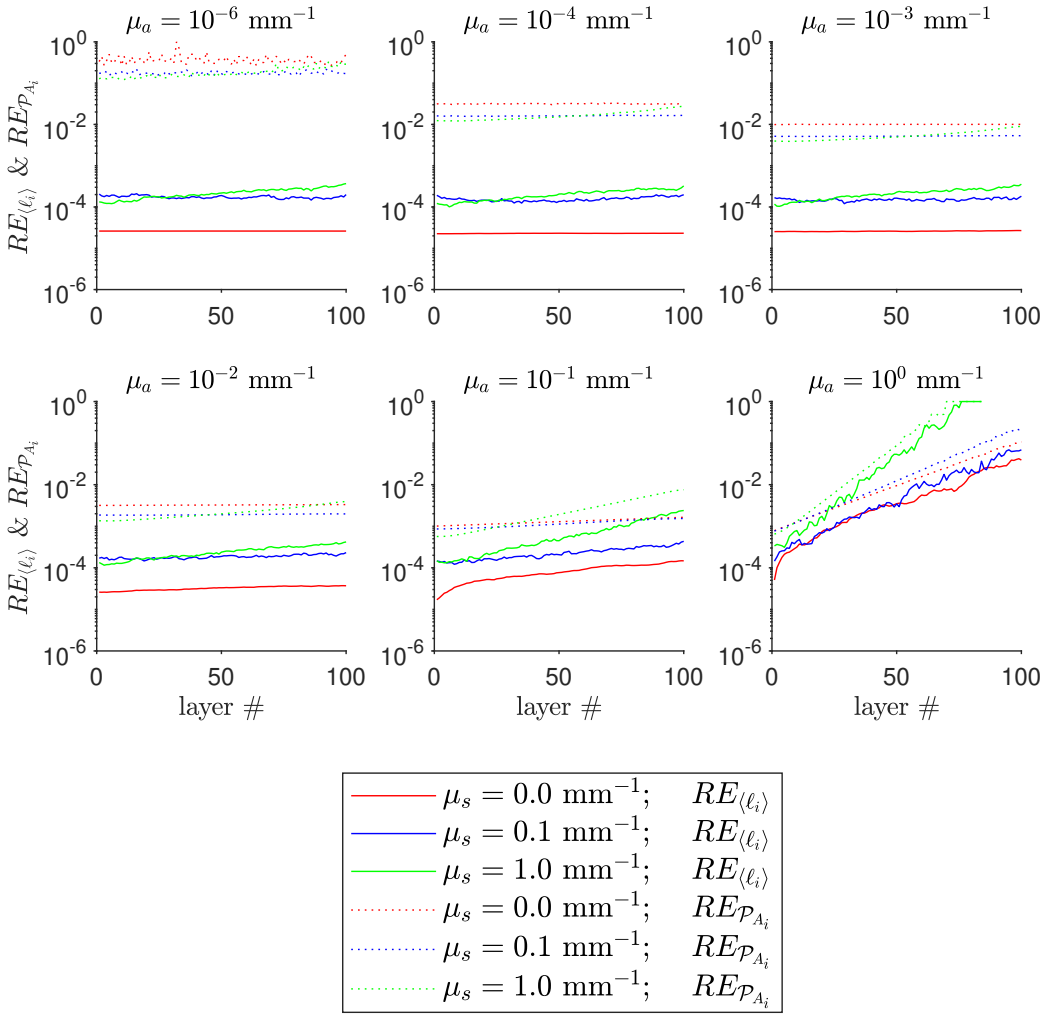

Figure 3. Relative errors $RE_{\mathcal{P}_{A_i}}$ and $RE_{\langle \ell_i \rangle}$, on the calculated fluence $\langle \Phi_i \rangle_{\mathcal{P}_{A_i}}$ and $\langle \Phi_i \rangle_{\langle \ell_i \rangle}$, computed with the ABM method and the PBM method, respectively, as a function of the layer number #. The range for the abscissa (ordinate) axis is the same for all the panels and the results pertain to $N = 10^8$.

reliability of the presented results we also notice that the the employed code has been accurately verified by previous investigations.[22,26]

Finally, we note that, although the presented MC results were obtained by using a Henyey-Greenstain scattering function with asymmetry factor $g = 0.8$, similar results are expected for any other kind of scattering function and distribution of the optical properties (μ_a, μ_s).

4. CONCLUSIONS

In conclusion, we have introduced a useful elementary formula, i.e., Eq. (2), valid in complete generality within the steady state RTE, to obtain the mean fluence rate, in a given sub-volume of a propagating medium, with a method (PBM) alternative to the classical one (ABM) usually utilized in NIRS. This method is based on the calculation of the mean pathlength traveled by all emitted photons inside a sub-volume of any shape, size and optical properties. As it can be deduced from the theory and the presented examples, the PBM can be easily implemented in any MC simulation for photon transport.

A potential advantage of the PBM is that it can improve the statistics and thus the convergence of the MC simulations. In fact, when measuring the mean pathlength (PBM), all the photons (paths) that cross the region of interest are taken into account. With the classical approach (ABM), only the "absorbed" photons are considered, and this may produce (especially for lower values of the absorption coefficient) a poorer MC statistics for the same number of launched photons. However, it remains to verify if the use of other MC methods for photon propagation (Microscopic Beer-Lambert law, Albedo-weight, Absorption and Scattering pathlength rejection method[24]) and especially their GPU implementations can confirm the results here obtained with the albedo rejection method. Further work it is in progress on these points and the preliminary results (data not shown) confirm that the advantages of the PBM still holds with other MC methods and also when PBM is implemented in a GPU environment as it is common in many open source codes nowadays available. Moreover, the PBM method can be also applied when the absorption coefficient is not constant or nil inside the considered sub-volume, whilst the applicability of the ABM method is not possible under these conditions.

A detailed proofs on the validity of Eq. (2) can be found in Ref. 19. It can be also worth to note that the validity of this relation is implicit inside the definition of radiance and fluence rate in the CW RTE.

Finally, we believe that the PBM method is based on a fundamental law that maybe should be better considered in biomedical optics given it general validity and its transparent simplicity. Thus, we hope that the awareness of this relation can help to fill a missing part on this interesting topic, and that it can also give a stimulus to develop original MC investigations related to biological tissues. It can be at last expected that the validity of the proposed relation between fluence and mean pathlength is also verified in a regime of anomalous transport.[27]

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