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Heuristic Model for Photon Propagation in Two-Layer Turbid Media

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Abstract: We propose a heuristic model for light propagation in two-layer turbid media, that accurately reproduces photon Distributions of Time-Of-Flight, while being faster than a full Monte Carlo approach, and is easily scalable to multi-layer domains.

1. Introduction

Accurately modelling photon propagation in two-layer domains proves useful in a wide range of *in-vivo* scenarios where tissue stratification makes it hard to justify the use of a simple homogeneous model. A few examples are extracerebral tissue over brain [1] or fat over muscle [2].

Currently available approaches for calculation of the photon Temporal Point Spread Function (TPSF) include Diffusion Equation (DE) analytical solutions or Monte Carlo (MC) simulations. While the former method provides unreliable results outside of the diffusion approximation, i.e. modest absorption values and sufficiently large source-detector distances, the latter is exact but rather taxing both in terms of computational time and storage space.

In fact, the conventional way of producing an exact DTOF for a two-layer structure via MC consists of performing a simulation on a white (absorption-less) domain and then perform weighted binning of all the simulated photon paths, exploiting the microscopic Beer-Lambert-Bouger law. Of course, such practice entails saving in a look-up table and retrieving all the partial pathlengths (PP) travelled by each photon in each layer of the medium [3], quickly leading to a huge increase in memory space requirements with the number of simulated photons and number of layers of the medium.

The approach we propose stems from found theoretical foundations as the Beer-Lambert-Bouger law and the Central Mean Theorem [4] and allows the retrieval of the $TPSF$ for a two-layer domain employing a simple rescaling of the white $TPSF_0$ of a two-layer medium, where absorption coefficients μ_{a0} and μ_{a1} of the upper and lower layers, respectively, are null.

$$TPSF(t) \approx TPSF_0(t|\mu_{a0} = \mu_{a1} = 0) \cdot \exp\left(-\mu_{a0}\langle \tilde{l}_0(t)\rangle\right) \cdot \exp\left(-\mu_{a1}\langle \tilde{l}_1(t)\rangle\right) \tag{1}$$

The exponential scaling terms contain the average PP of photons with arrival time t, travelled in the upper layer $\langle \tilde{l}_0(t)\rangle$ and in the lower layer $\langle \tilde{l}_1(t)\rangle$ of a medium with absorption coefficients of the layers equal to $\frac{\mu_{a0}}{2}$ and $\frac{\mu_{a1}}{2}$, respectively.

Scalability to multi-layer gometries is achieved by inserting as many exponential terms of the kind $\exp\left(-\mu_{ai}\langle \tilde{l}_i(t)\rangle\right)$ as the number of layers.

By comparing TPSFs calculated with (1) to those obtained from a full MC approach, we aim to prove that our heuristic formula provides good accuracy of the reconstructed curve, even in challenging regimes where the diffusion approximation struggles, while significantly reducing the time and stored information needed for computation.

2. Materials and methods

MC simulations were run on the GPU accelerated light transport simulator MCX [5], starting from white simulations and performing weighted binning with the partial pathlengths of each photon to produce exact MC TPSFs. In this instance, we also retrieved the white $TPSF_0$ and average PP $\langle \tilde{l}_0(t)\rangle$ and $\langle \tilde{l}_1(t)\rangle$, necessary for the application of (1).

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We considered a two-layer semi-infinite medium made up of a superficial (upper) layer of variable thickness s_0 from 2 mm to 8 mm and a bulk (bottom) layer of fixed thickness $s_1 = 40$ mm. Refractive indices of the layers are identical and equal to 1.4, with air as external medium, null anisotropy factor and a source-detector distance of $\rho = 10, 20$ mm. Multiple combinations of reduced scattering coefficients μ'_{s0}, μ'_{s1} and absorption coefficients μ_{a0}, μ_{a1} were considered, either equal or different between the layers.

Moreover, the following benchmark to show the advantages of the method in terms of computational speedup and storage space was conceived.
The same geometry described above, with $s_0 = 4$ mm, $\mu'_{s0} = 1$ mm^{-1}, $\mu'_{s1} = 0.5$ mm^{-1} and $\rho = 10$ mm was employed. The simulation was repeated for five different target values of detected white photons $N_{target} = 10^6, 5 \cdot 10^6, 10^7, 5 \cdot 10^7, 10^8$ and the partial pathlengths of all photons in both layers were saved as exact MC datasets. Moreover, for each of the five simulations, the white $TPSF_0$ was binned ($N_{bin} = 200$ temporal bins, 10 ps bin width) and mean pathlengths for upper and lower layer were calculated for each of $N_{abs}^2 = (10)^2$ combinations of absorption coefficients of the two layers to reconstruct. Specifically, the 10 chosen absorption values are equally spaced and span from 0.01 mm^{-1} to 0.055 mm^{-1}. The white $TPSF_0$ together with the mean PP amount to the heuristic dataset and allow to reconstruct the $TPSF$ according to (1).
For each of the five simulations, we estimated the time required to read the whole exact MC dataset and calculate the 100 $TPSF$'s accounting for absorption of both layers via photon-by-photon weighted binning. We compared this time to the time required to load the heuristic dataset and calculate the same 100 curves via (1). The calculations were run using MATLAB on an Intel® Xeon® Processor E5-2670 v3 @2.30 GHz, 192 GB RAM @2133 MHz.

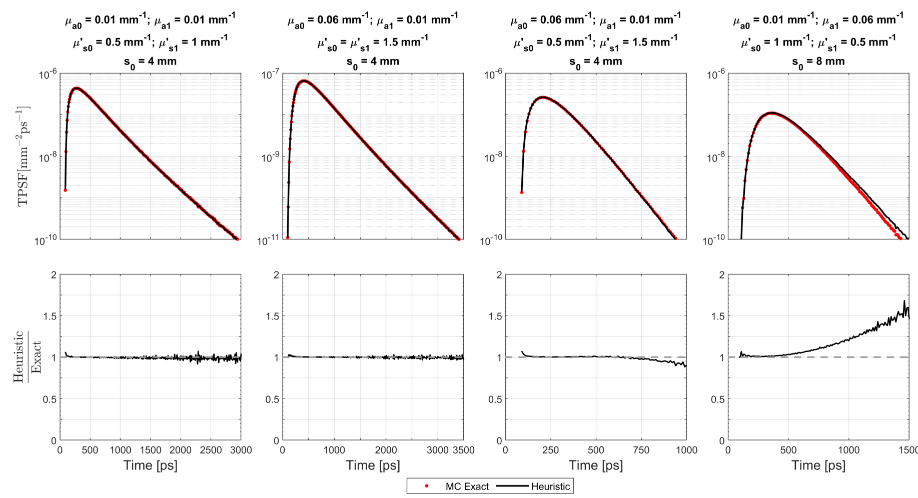

Fig. 1: Top row: comparison of the $TPSF$ obtained in a two-layer medium in reflectance geometry using the heuristic approach (black line) and MC simulation (red line). Bottom row: ratio of the heuristic to the exact $TPSF$. Common parameters: thickness of bottom layer $s_1 = 40$ mm, refractive indices $n_{ext} = 1$ and $n_0 = n_1 = 1.4$, isotropic scattering, source-detector distance $\rho = 20$ mm. The optical properties of both layers and the upper layer thickness are specified in the header of each column.

3. Results and discussion

A few relevant comparisons between heuristic and exact MC methods are presented in Fig.1. In all cases, the error at early times (< 500 ps), intended as the ratio between heuristic and exact $TPSF$ at a given time point is negligible, increasing to up to 10% at late arrival times. In the fourth column, the error on the tail reaches 50%, due to the significant nonlinearity of the average PP at late times with respect to the absorption coefficient, that is a fundamental requisite for the viability of the heuristic method [4].

Fig.2 shows how the computation time of the curves for the two methods and the dimensions of their respective datasets used for such calculation grow with the target number of detected white photons set for the given simulation.
Of course, heuristic dataset size is independent from N_{target}, since it scales as the sum of two contributions, one related to the $TPSF_0$ and the second relative to the mean PP, yielding the proportionality:

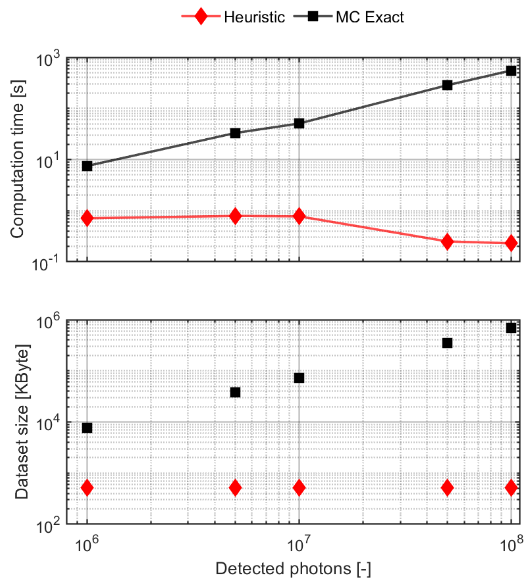

Fig. 2: Heuristic model vs. MC exact simulations: scaling behavior with respect to the target number of detected white photons. Top row: computation time for 100 colored $TPSF$s with various combinations of absorption coefficients in the two layers. Bottom row: size of the dataset required to compute the benchmark $TPSF$s.

$$Heur\,Dataset\,Size \propto N_{bin} + N_{layer} \cdot N_{abs}^{N_{layer}} \cdot N_{bin} \approx N_{bin} \cdot N_{abs}^{2} \tag{2}$$

Comparatively, for a two-layer medium, the size of the exact MC dataset depends linearly on N_{target} as $N_{layer} \cdot N_{target}$, where $N_{layer} = 2$ for a two-layer structure and equal to the number of layers in a multi-layer domain.

When implementing inversion procedures involving numerical models like MC, it is advisable to operate with a sufficiently high number of detected white photons for guaranteeing a sufficiently smooth model. For example, in the case of $N_{target} = 10^{7}$, the dataset dimensions are 74 MBytes for the exact MC and 515 KBytes for the heuristic one, translating into a 70-fold decrease in computation times from 50.70 s to 0.77 s in favor of the heuristic method.

4. Conclusions

The proposed heuristic approach offer more than reasonable accuracy in the description of photon propagation through two-layer media, with deviations from the ideal behavior only in conditions of extreme differences of absorption and scattering between the layers.
The swiftness in the calculation of the $TPSF$ and low size of look-up dataset make it promising for implementation in inversion procedures, where multiple computations of the model are required and the look-up dataset also needs to account for various combination of scattering values of the layers, further expanding its size.

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