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Importance Sampling based Monte Carlo simulation of time domain optical coherence tomography with embedded objects

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Monte Carlo simulation for light propagation in biological tissue is widely used to study light-tissue interaction. Simulation for optical coherence tomography (OCT) studies require handling of embedded objects of various shapes. In this work, time-domain OCT simulations for multi-layered tissue with embedded objects (such as sphere, cylinder, ellipsoid, and cuboid) was done. Improved importance sampling (IS) was implemented for the proposed OCT simulation for faster speed. At first, IS was validated against standard and angular biased Monte Carlo method for OCT. Both Class I and Class II photons were in agreement in all the three methods. However, importance sampling method had more than ten-fold improvement in terms of simulation time. Next, B-scan images were obtained for four types of embedded objects. All the four shapes are clearly visible from the B-scan OCT images. With the improved importance sampling B-scan OCT images of embedded objects can be obtained with reasonable simulation time using a standard desktop computer. User friendly, C based, Monte Carlo simulation for tissue layers with embedded objects for OCT (MCEO-OCT) will be very useful for time domain OCT simulations in many biological applications. © 2016 Optical Society of America

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1. INTRODUCTION

Optical coherence tomography (OCT) is a non-ionizing and noninvasive optical imaging modality with many biomedical applications. OCT system produces high-resolution, cross-sectional tomographic images by acquiring the backscattered or backreflected light from various layers of the tissue [1]. This reflectivity profile contains information about the spatial dimensions and location of structures within the tissue. Sample is excited with super-luminescent diodes (or semiconductor diode) emitting low-coherent and extremely short laser pulses (few hundreds of femtosecond). The light reflected back by the scattering medium (biological tissue) has the information of time of flight, which contributes to the spatial resolution [2-4]. Resolution of OCT imaging systems are 1-15 μm . Axial resolution is mainly dependent on the coherence length, and bandwidth of the excitation source [5]. OCT has higher depth of penetration in biological tissue compared to other pure optical imaging modality, such as two photon microscopy [6, 7]. Imaging depth in OCT is confined to 1-3 mm in tissue. OCT is potentially a powerful tool used for cross-sectional in vivo imaging of ocular tissue to detect and monitor macular diseases

[8]. It is widely used in retinal imaging [9, 10]. OCT also has the ability to acquire skin images [11, 12]. Recently, applications of OCT has been extended to study neurological diseases [13]. Examples of other OCT applications are stent imaging, imaging of sentinel lymph node biopsies and in vivo imaging of oral cavity [14-16].

OCT system is developed on the principles of Michelson interferometer [3]. Based on the bandwidth of excitation source and means of detection of reflected light, OCT imaging systems are divided into time domain and frequency domain OCT system [17]. In this work, we will focus all our discussion on time domain OCT. Light from a super luminescent diode (low-coherent), the commonly used illumination source, is either used in free-space or coupled in to single-mode fiber. The incident light is split to the reference arm (usually a mirror) and the sample arm (target sample, i.e., tissue). The light reflected from both the arms reach the detector (photodiode). The light reflected back from the reference arm and the sample arm interferes coherently if they have "same" optical path-length ("same" meaning a difference of less than a coherence length). Scanning of the mirror in the reference arm produces a reflectivity profile of the sample (called A-scan or A-line scan).

Areas of the sample that reflect back a lot of light will give rise to stronger interference than areas that don't. Any light that is outside the short coherence length will not interfere. Laterally combining a series of axial depth scans (A-scans) produces a cross sectional tomograph (B-scan) [18].

Design of excitation source and collecting fiber for any of the optical imaging modality requires understanding of light propagation in tissue. Monte Carlo simulations are the gold standard to study the interaction between light and tissue [19]. In OCT simulation, relationship between path-length resolved signal and OCT signal was given based on linear system theory, and Huygens-Fresnel diffraction optics [20-22]. Monte Carlo simulations were also done to study the OCT signal from turbid homogenous medium [23-25]. Standard C based Monte Carlo simulation for light propagation in multi-layered tissue (MCML) [26] was modified, for faster simulation of class I (signal) and class II (noise) photons at a given probing depth [27]. In this work, MCML for OCT was accelerated by angle biased scattering of photons that reach the probing depth, which ensures more number of photons reach the collecting fiber. Photons that are angle biased are subjected to weight reduction for statistical

equivalence. The main drawback of angle-biased scattering is that the simulation is done for each probing depth leading to increased simulation time for an A-line OCT scan or a B-scan OCT image. To overcome this drawback, importance sampling (IS) was proposed to calculate the OCT signal in a multi-layered tissue medium [28]. In IS, photons were biased to the direction of the collecting fiber, and the likelihood ratio of biased and unbiased scattering was computed to modify the weight of the photon accordingly. Since the photons undergo biased scattering at the first scattering site, the strength of the class II signal was weak. They further improvised the importance sampling with randomization of biased sampling which required modification of the generation of biased angle [29].

Various simulation geometries have been explored in the literature. Multi-layer tissue structure is very common in many light-tissue interaction simulations due to its simplicity. Multi-layered tissue with embedded objects was also modelled to simulate more realistic tissue structures [30-32]. Simulation of blood vessel using mesh based Monte Carlo (MMC) was developed for image generation of angiographic OCT [33]. Improved importance sampling was also combined with MMC

Fig. 1. Flowchart for MCEO-OCT based on improved importance sampling. $z_{\max}$ is maximum depth reached by the photon, s is step-size, d_b is distance to boundary, μ_t is extinction coefficient, opl_i is optical path length, z_i is the current depth of photon, $r_{\max}$ and $\Phi_{\max}$ are the radius and acceptance angle of collecting fiber, r_i and Φ_i are the current distance of the photon from fiber center and the angle between photon and fiber-axis, d is the probing depth, w_i is the weight of the photon, L_i is the likelihood ratio, l_c is the coherence length, and p is the probability of biased scattering.

for simulation of OCT signals with arbitrary spatial distributions [34]. The computational cost (in terms of memory and time) of MMC simulations are higher than C based MCML due to the dependence of MMC on MATLAB [35]. They also depend on graphical processing units and CUDA programming languages for speed and real-time applications [36]. Therefore, there is a need for developing fast C based Monte Carlo to simulate OCT for tissue structure with embedded objects.

In this work, a more efficient MCML-OCT with embedded objects is reported. MCML-EO (which simulates light propagation in tissue with embedded geometric shapes) was modified for MCEO-OCT with improved importance sampling (to accelerate the computation of class I and class II photons) [35]. Photon-boundary interaction of simple geometries, such as sphere, ellipse, cylinder, and cuboid can be checked by ray-plane equations. Hence, complex mesh based geometry is not needed in this approach. At first, IS was validated against standard and angular biased Monte Carlo method for OCT. Next, B-scans OCT images were obtained for four types of embedded objects using MCEO-OCT.

2. Improved importance sampling for MCEO-OCT

A. Monte Carlo modelling of light propagation

Light propagation in multilayered tissue (MCML) is simulated by tracking photon packets in the medium based on its optical properties [26]. Absorption coefficient (μ_a), scattering coefficient (μ_s), scattering anisotropy (g) of the given medium determine the trajectory of the photon packets. The photon packet of weight (w) is launched in the medium at a position [typically origin (0,0,0)] with a photon propagation direction [typically normal incidence to the medium is considered (direction cosines in the respective axis $u_x = 0$, $u_y = 0$, and $u_z = 1$)]. The step-size (s), determined by the random number (ξ) generated for each step and the medium's extinction coefficient ($\mu_t = \mu_s + \mu_a$), is given as $s = -\ln(\xi)/\mu_t$. Once the photon moves (by the distance s) to the scattering site, it undergoes absorption. Absorption is the process in which the photon weight is dropped [$\Delta w = (\mu_a/\mu_t) * w$]. The weight dropped is recorded in a 2-dimensional grid across depth (z) and radial directions. After absorption the photon undergoes the next scattering event. To do so, the new scattering direction is determined as follows. The probability distribution function for the new scattering angle θ in polar co-ordinate system is given by the Henyey-Greenstein function (f_{HG}) as,

$$f_{HG}(\cos\theta) = \frac{1 - g^2}{2(1 + g^2 - 2g\cos\theta)^{3/2}} \quad (1)$$

Tracking of the photon packet ends when its weight is less than the threshold (10^{-6}) using Russian roulette or when it escapes the simulation geometry boundaries. Russian roulette gives the photon of weight (W) one opportunity to survive in m times (say 10 times) with a weight of mW . Distance between the photon and the boundary (d_b) is checked at each scattering site. If the photon is escaping to the ambient medium, then it is recorded as diffused reflectance (when the photon comes out from the photon launching side) or diffused transmittance (otherwise).

B. Monte Carlo modelling for optical coherence tomography

Class I photons in OCT are the diffuse reflectance photons which are reflected/scattered from the target layer (z') whose thickness is $[l_c/(2n)]$, where l_c is the coherence length of the light source in vacuum, and n is refractive index of the simulating medium. All our work is done using $n=1$, therefore we will ignore n in all the equations hereafter. The probing window is $[(d - l_c/2), (d + l_c/2)]$ where d is the probing depth (reference arm optical path-length). That means the optical path-length of these photons reflected back from the probing depth must be within the range $[(d - l_c/2), (d + l_c/2)]$. Class II photons are the photons that have undergone multiple scattering, but still interfere with the reference arm light. That means their optical path-length is also within the range $[(d - l_c/2), (d + l_c/2)]$, but they have not entered the target depth. The class II photons are the noise in the OCT signal. Since, the scattering anisotropy g is close to 1 for biological tissue, the photons are mostly forward scattered. As a result the number of photons reaching the launch surface (back-scattered) are quite low. To obtain statistically significant class I and class II photons one requires OCT simulation with very large number of photon packets. This leads to increase in the simulation time for obtaining single A-line OCT signal. Simulations for B-scan OCT is even more time consuming and practically not feasible, as single B-scan image will have tens to hundreds of A-line OCT data.

Fig. 2. Unbiased (a) and biased (b) scattering event at the scattering site for improved importance sampling. u - Propagation direction of the photon, v_{ub} - Scattered direction during unbiased scattering, f - Direction towards the collecting fiber, θ_s - Scattering angle sampled by Henyey-Greenstein function (Eq. 3), θ'_B - Angle between f and v_{ub} , v_b - Scattered direction during biased scattering, θ_B - Scattering angle sampled by biased probability density function (Eq. 5), θ'_s - Angle between u and v_b .

C. Angle Biased Monte Carlo

To overcome this challenge, an angle biased sampling was proposed [27]. Here, an artificially biased scattering phase function was used to replace the true phase function when sampling the scattering angle, and then the weight of the photon is also compensated [37]. The artificial phase function used was $f_{HG}(-\cos\theta)$, instead of $f_{HG}(\cos\theta)$ as in Eq. 1. That means after $\cos\theta$ is sampled using the Henyey-Greenstein

function (f_{HG}) in Eq. 1, $-\cos\theta$ is actually used to calculate the direction of travel of the photon packet. The photon weight (w) is compensated by,

$$\bar{w} = \left(\frac{1 + g^2 + 2g\cos\theta}{1 + g^2 - 2g\cos\theta} \right)^{3/2} w \quad (2)$$

This significantly reduced the computation time. However, the drawback of the angle-biased scattering is that the biasing is done only when the photons reach the target depth, so one needs to run the simulation for each target depth to compute a A-line scan. In spite of reduction in simulation time for a single probing depth, angle-biased method still takes large amount of computation time for simulating the entire A-line scan. Further, obtaining B-scan OCT images using this method is still not very practical.

D. Improved Importance Sampling (IS) Monte Carlo

To accelerate MCML for OCT further, an improved importance sampling based algorithm was proposed [28, 29]. Here also biased scattering and photon weight compensation was used like the angle-biased method. However, there are some significant changes the way it was done. The site of the first biased scattering is randomly chosen and the weight of the photon is reduced accordingly based on a likelihood ratio while recording. The modifications of MCML for improved importance sampling are highlighted in the flowchart given in Fig. 1. The decision on whether a photon packet undergoes a biased or an unbiased scattering is taken statistically with a probability of p . The probability of biased scattering is p and $(1 - p)$ is the probability of unbiased scattering. First, a random number (ξ) is selected, if $\xi < p$, then the photon undergoes biased scattering, otherwise it undergoes normal unbiased scattering ($\xi > p$). For an unbiased scattering event (Fig. 2a), the scattering angle $\cos\theta_s$ is computed [from Henyey-Greenstein function (f_{HG}) in Eq. 1] as,

$$\cos\theta_s = \left(\frac{1}{g} \right) \times \left\{ 1 + g^2 - \left(\frac{1 - g^2}{1 - g - 2\xi} \right)^2 \right\} \quad (3)$$

where, ξ is a random number. If the photons current propagation direction is u , then the new propagation direction v_{ub} is updated based on $\cos\theta_s$. This means $\cos\theta_s = u \cdot v_{ub}$. Once the direction cosines of the photons are updated, then the angle between the new propagation direction v_{ub} and the Direction to Fiber (f) is computed to obtain θ'_B ($\cos\theta'_B = f \cdot v_{ub}$). θ'_B is needed for the calculation of likelihood ratio, which will be discussed later.

In case the photon undergoes biased scattering (Fig. 2b), the scattering phase function used is (different from Henyey-Greenstein function),

$$f_B(\cos\theta_B) = \left(1 - \frac{1-a}{\sqrt{a^2+1}} \right)^{-1} \times \frac{a(1-a)}{(1+a^2-2a*\cos\theta_B)^2} \quad (4)$$

where, a is the given bias coefficient in the range $[0, 1]$. Thus, the biased scattering angle $\cos\theta_B$ is computed from Eq. 4 as,

$$\cos\theta_B = \left(\frac{1}{2a} \right) \times \left\{ a^2 + 1 - \left[\xi \left(\frac{1}{1-a} - \frac{1}{\sqrt{a^2+1}} \right) + \frac{1}{\sqrt{a^2+1}} \right]^{-2} \right\} \quad (5)$$

Note that, the photon's new propagation direction (v_b) is at an angle θ_B with respect to the Direction to fiber (f). Thus, $\cos\theta_B = f \cdot v_b$. Once the direction cosines of the photons are updated, then the angle between the new propagation direction (v_b) and the original photon propagation direction (u) is computed to obtain θ'_s ($\cos\theta'_s = v_b \cdot u$). θ'_s is needed for the calculation of likelihood ratio, which will be discussed next. The likelihood ratio calculated at each scattering site as

$$L(\cos\theta) = \frac{f_{HG}(\cos\hat{\theta}_s)}{p * f_{HG}(\cos\hat{\theta}_s) + (1-p) * f_B(\cos\hat{\theta}_B)} \quad (6)$$

where, $\hat{\theta}_s = \theta_s$, $\hat{\theta}_B = \theta'_B$ for unbiased scattering; and $\hat{\theta}_s = \theta'_s$, $\hat{\theta}_B = \theta_B$ for biased scattering. Likelihood ratio at each scattering site is multiplied to compensate for the weight of the photon. The product of likelihood ratio (L) is initialized to 1 while launching the photon.

Fig. 3. Simulation set-up. (a) 1 mm thick uniform layer, (b) 1 mm thick multilayer set-up with 4 layers of thickness 15 μm is embedded at depths 200, 645, 760 and 900 μm . Also a layer of 30 μm was embedded at depth 365 μm . (c-f) 1 mm thick simulation geometry with embedded object - sphere, cylinder, ellipsoid, and cuboid. All four objects are located at a depth 0.2 mm. Sphere has a diameter of 0.2 mm; cylinder has diameter 0.2 mm and infinite length along x-axis; the ellipse has radius of 0.13 mm, 0.08 mm, and 0.01 mm along x-, y-, and z-axis, respectively; cuboid has of length of 0.26 mm, breadth 0.15 mm, and height 0.2 mm in x-, y-, and z-axis, respectively. Inset is the table giving the optical properties of the simulation set-up.

At each scattering site, the optical path length (opl_i) of the current photon (i^{th}) is updated. In order to track the maximum depth reached by the photon, z_{max} is updated with the current depth of the photon (z_i) if the photon is currently at a deeper position than the present value of the z_{max} . Both opl_i and z_{max} are initialized to 0, during the launch of the photon. At every scattering site z_{max} is updated as follows,

$$z_{max} = \begin{cases} z_i, & \text{if } z_i > z_{max} \\ z_{max}, & \text{otherwise} \end{cases} \quad (7)$$

Once the photon reaches the launch surface, spatial and temporal filtering is done to record the class I and class II photons. To ensure the i^{th} photon is within the reach of collecting fiber, its radial distance from the fiber center (r_i) should be within the radius of the collecting fiber (r_{max}). The angle of emitting photon with the fiber axis (Φ_i) has to be within the acceptance angle of the fiber (Φ_{max}). Temporally to check if the photon is within the probing depth, the condition ($|opl_i - 2z'| < l_c/2$) is to be satisfied, where, z' is the probing depth. The probing depth z' ranges from 0 to thickness of simulation medium for our experiments. On the satisfaction of the aforementioned three conditions, it is ensured that the photon contributes to OCT signal. To classify the photon further, on satisfaction of $|opl_i - 2z_{max}| < l_c/2$, the photon is recorded as class I photon, otherwise it is recorded as class II photon. During the recording, the product of likelihood ratio (L_i) and weight (W_i) of the photon is multiplied and recorded as either class I or class II photons. OCT class I (R_1) and class II (R_2) diffuse reflectance, recorded at depth z' for the (i^{th}) photon is given by Eq. 8.

$$R_{1,2}(z') = \frac{1}{N} \sum_{i=1}^N I_{1,2}(z', i) * L_i * W_i \quad (8)$$

where, N is the number of photon packets and I_1 and I_2 are the spatial and temporal filter for class I and class II photons. Filters to classify the i^{th} photon into class I or class II is given in Eq. 9 and Eq. 10,

$$I_1(z', i) = \begin{cases} 1, (l_c/2) > |opl - 2z_{max}|, r_i < r_{max}, \\ \Phi_i < \Phi_{max}, |opl - 2z'| < (l_c/2) \\ 0, otherwise \end{cases} \quad (9)$$

$$I_2(z', i) = \begin{cases} 1, (l_c/2) < |opl - 2z_{max}|, r_i < r_{max}, \\ \Phi_i < \Phi_{max}, |opl - 2z'| < (l_c/2) \\ 0, otherwise \end{cases} \quad (10)$$

3. Simulation set-up

All simulations were run using a desktop computer with Intel Xeon 3.7 GHz 64-bit processor and 16 Gb RAM running windows operating system. ANSI standard C code of MCML used in this work [26]. For standard MCML runs, modification were done for recording (spatial and temporal filtering was incorporated) of class I and class II photons. For improved importance sampling based simulations, the scattering event is modified. All the parameters needed for the simulations are listed in Table 1. The simulation output is written into a text file. Class I and class II photons for each depth grid was recorded. **For OCT of embedded objects the MCEO code [35] was modified to incorporate improved importance sampling.** Table 1 lists all the input parameters required to run the simulation.

To validate the importance sampling based MCML-OCT, IS results were first compared against the standard angle biased MCML (AB), and standard MCML (STD) simulation results for a uniform tissue layer of thickness 1 mm (Fig. 3a). Next, a multi-layer simulation geometry was considered with 4 layers of thickness 15 μm embedded at depths 200, 645, 760 and 900 μm . Also a layer of 30 μm was embedded at depth 365 μm (Fig.

3b). For this simulation setup IS and STD MCML was simulated, and the results were compared. These two simulation setups were used to confirm that the IS method provides same results compared to gold standards with significantly lesser simulation time.

Table 1 List of all the input parameters, its notations, and values set for the simulation study of layered and embedded object

Parameter	Symbol	Value
Number of photons	N	IS-objects - 10^9 IS-layer - 5×10^9 AB - 10^9 STD - 10^{11}
Recording grid resolution along z-axis	dz	5 μm
Number of grids along z-axis	nz	200
Coherence length	l_c	15 μm
Collecting fiber radius	r_{max}	10 μm
Collecting fiber acceptance angle	Φ_{max}	5°
Absorption coefficient	μ_a	Background: 1.5 cm^{-1} Insertions: 3.0 cm^{-1}
Scattering coefficient	μ_s	Background: 60 cm^{-1} Insertions: 120 cm^{-1}
Scattering anisotropy	g	0.9
Refractive index	n	1
Biasing coefficient	a	0.9
Probability of biased scattering	p	0.5
For B-scan		
Start of scan along x-axis	-	-0.015 cm
End of scan along x-axis	-	0.015 cm
Number of A-lines for a single B-scan	-	50
Embedded objects		
Center of the object	-	(0,0,0.2) mm
Sphere	-	Radius: 0.1 mm
Cylinder	-	Radius: 0.1 mm, infinite length along x-axis
Ellipsoid	-	Radius along x, y, and z axis: 0.13 mm, 0.08 mm, and 0.1 mm
Cuboid	-	Length (x), breadth (y), and height (z): 0.26 mm, 0.15 mm, and 0.2 mm

Next, MCEO-OCT is computed for four embedded objects – sphere, cylinder, ellipse, and cuboid of thickness (along z-axis) 0.2 mm centrally located at a depth of 0.2 mm. Sphere is of radius 0.1 mm is shown in Fig. 3c. The cylinder with diameter 0.2 mm (Fig. 3d) has infinite length (along x-axis). The ellipse has radius of 0.13 mm, and 0.08 mm along x- and y-axis, respectively (Fig. 3e). Similarly, cuboid (Fig. 3f) has length of 0.26 mm and breadth 0.15 mm in x- and y-axis, respectively. 50 A-line scans are done from -0.15 mm to 0.15 mm along x-axis to form the B-scan OCT image. The embedded layers and embedded objects are the shaded regions in Fig. 3.

4. Results and discussion

First the implementation of modified IS MCML is compared against the angle biased MCML (AB) and standard MCML (STD) simulations with simple single layer or multi-layer simulation geometry. Fig. 4(a) shows the results for an 1 mm thick single layer simulation geometry. It is clearly seen that the IS is able to produce both class I and class II photons similar to the AB and STD simulations. The noise in AB class II photons (dotted-dashed green line) is higher compared to class II photons from STD (black dashed line) and IS (solid red line). The correlation of class I and class II photons for the three methods validates the correctness of modified IS based MCML-OCT. Note that, the modified IS simulation was run with 5×10^9 photons, whereas AB and STD were run with 10^9 and 10^{11} photons, respectively. This resulted significant savings in terms of computation time. Time taken for IS, AB, STD MCML simulations were 6, 42, 75 hours, respectively. Time taken by modified importance sampling is less by one-tenth the standard MCML and one-seventh of the angular biased MCML for OCT.

Fig. 4. (a) Comparison of the simulation results from modified importance sampling MCML simulation (IS), angle biased MCML (AB) and standard MCML simulation (STD) for OCT for the single layer simulation geometry (Fig. 3a). (b) IS and STD simulations for OCT for multi-layer set-up (Fig. 3b). In both the cases class I and class II photons are shown. STD was run for 10^{11} photons whereas IS was run only for 5×10^9 photons. AB was also simulated for 10^9 .

Fig. 5. A-line scans of class I and class II photons for the MCEO-OCT simulations. (a) class I photons of embedded objects, (b) class II photons of embedded objects, (c) class I and class II photons of embedded objects combined in the same plot, plot shown only up to a depth of 0.5 mm.

Next, a 1 mm thick multi-layered simulation geometry was used (Fig. 3b). Fig. 4b shows the simulation results for the IS and STD MCML OCT. IS and STD simulations were run with 5×10^9 and 10^{11} photons, respectively. As expected both Class I and Class II photons matches quite well. Class I photons (dashed red line) from STD are comparatively noisy beyond the depth of 0.4 mm. Class II photons (dashed green line) is noisy throughout the simulation depth. A noticeably broad peak is seen in class I curves around the second embedded layer which is of thickness $30 \mu\text{m}$. Beyond 0.5 mm the class II photons are more than the class I photons in both uniform layer and multi-layer simulation geometry. For the multi-layer set-up simulation of STD MCML OCT took 103 hours and IS MCML OCT took only 7 hours. There is more than 14 times improvement in the computation time with IS method.

Once the validation of IS MCML-OCT was complete in comparison with the STD and AB MCML-OCT method, we run the simulation for IS MCEO-OCT for the embedded objects. Four objects (sphere, cylinder, ellipse, and cuboid) were embedded in the simulation geometry and IS MCEO OCT was run. Fig. 5 is the A-line scan of the embedded objects along the origin. Class I photons (Fig. 5a) of all four objects resemble each other. Class II (Fig. 5b) photons are also similar across four objects. As observed in Fig. 5c, class II photons exceeds class I at depth greater than 0.4 mm which is similar to the trend seen in multilayer simulations. It is challenging to study the geometry of the embedded objects from single A-line scan. Hence, multiple A-line scans were acquired with a lateral step size of $6 \mu\text{m}$ to form the B-scan OCT image. Note that, the lateral step size selected was roughly one fourth of the collecting fibre diameter ($20 \mu\text{m}$). Fig. 6 shows the B-scan images of class I and class II photons of the embedded objects for the whole probing

Fig. 6 Simulated class I and class II reflectance-based B-scan OCT images obtained from MCEO-OCT simulations with improved importance sampling. a) For sphere, b) for cylinder, c) for ellipsoid, and d) for the cuboid. Also shown alongside is the zoomed view of the distribution of the respective class I and class II photons from 0 to 0.4 mm.

medium (0 to 1 mm). The class I and class II images are also zoomed between 0 to 0.4 mm for better view. The x-axis ranges from -0.15 mm to $+0.15$ mm in both, the complete images and zoomed in images. All the A-line simulations were run for 10^9 photons. Fig. 6a corresponds to the sphere and took a run-time of 54 hours. Fig. 6b corresponds to the cylinder with a run-time of 67 hours. Fig. 6c corresponds to ellipsoid with a run-time of 72 hours. Fig. 6d represents the cuboid with a comparatively longer run-time of 110 hours. The volume of cuboid (0.0078 mm³) being less than that of sphere (0.034 mm³) leads to less weight loss by photons in cuboid simulation geometry may be one of the reasons for increased simulation time for cuboid.

For all the simulations diffuse reflectance of class I photons is in the order of 10^{-6} and class II photons is two orders of magnitude less (in the order of 10^{-8}). Reflectance of class II overtakes the reflectance of class I photons beyond a depth of 0.2 mm for the optical properties of the simulation medium considered in this work. It is also to be noted that the geometry of embedded object is clearly decipherable from the B-scan of class I photon.

For a different multilayer set-up, MMC-IS based OCT takes approximately double (43 minutes) the time taken by C-based MCML-IS, which takes 24 minutes [34]. Here, OCT simulation of an embedded sphere (Figs. 6a) takes 54 hours for 50 A-line scans (approximately 65 minutes per A-scan) for 10^9 photons. Simulation of the sphere for 10^8 photons takes 5 hours for 50 scans. On using MMC-IS based simulation of embedded object, the computation time is 53 hours for 75 scans (approximately

42 minutes per A-scan) for 10^7 photons. MMC also takes a few seconds to minutes for the mesh generation depending on the mesh density and simulation volume [35]. **3D OCT simulation is also possible. Currently the fiber is scanned along one axis (x-axis) to generate a B-scan image. The fiber can be scanned in both axes (x and y) so that 3D volumetric OCT can be simulated. But for 3D simulation the total computation time will be significantly higher, therefore, it was not done in this work. However, we can parallelize the code with GPUs [30, 36, 38]. Thus, in the future with the help of faster computing 3D volumetric OCT simulation should be feasible with reasonable computing time.**

5. Conclusion

Time-domain OCT simulations for multi-layered tissue with embedded objects were done with improved importance sampling for faster speed. Improved importance sampling method was first validated against angle biased and standard Monte Carlo simulations for OCT. Simple single and multi-layered tissue geometry was used for the validation. Both Class I and Class II photons were in agreement in all the three methods. However, importance sampling method had more than ten fold improvement in terms of simulation time. Next, B-scans OCT images were obtained for four types of embedded objects (sphere, cylinder, ellipsoid, and cuboid). All the four shapes are clearly visible from the B-scan OCT images. With the improved importance sampling B-scan OCT images can be

obtained with reasonable simulation time using a standard desktop computer. For simple geometries this method will be much easier to use compared to mesh based Monte Carlo simulations for OCT. However, for complex geometries (irregular shapes) mesh based Monte Carlo method will be better. **Since the light propagation in tissue for time domain and frequency domain OCT is identical [17], the proposed simulation can be extended in the frequency domain OCT as well.**

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