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Raman Monte Carlo Simulation for light propagation for tissue with embedded objects

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ABSTRACT

Monte Carlo (MC) stimulation is one of the prominent simulation technique and is rapidly becoming the model of choice to study light-tissue interaction. Monte Carlo simulation for light transport in multi-layered tissue (MCML) is adapted and modelled with different geometry by integrating embedded objects of various shapes (*i.e.*, sphere, cylinder, cuboid and ellipsoid) into the multi-layered structure. These geometries would be useful in providing a realistic tissue structure such as modelling for lymph nodes, tumors, blood vessels, head and other simulation medium. MC simulations were performed on various geometric medium. Simulation of MCML with embedded object (MCML-EO) was improvised for propagation of the photon in the defined medium with Raman scattering. The location of Raman photon generation is recorded. Simulations were experimented on a modelled breast tissue with tumor (spherical and ellipsoidal) and blood vessels (cylindrical). Results were presented in both A-line and B-line scans for embedded objects to determine spatial location where Raman photons were generated. Studies were done for different Raman probabilities.

Keywords: Monte Carlo simulation, Raman imaging, embedded objects.

1. INTRODUCTION

Recently, optical imaging techniques which employ non-ionizing radiations have proven to be a valuable tool [1]. Optical imaging modalities such as photoacoustic (PA) imaging, fluorescence imaging, optical coherence tomography (OCT) and Raman imaging are widely used for non-ionizing imaging [1-5]. However, most of these optical imaging modalities are challenged with sufficient penetration depth. In each of these optical imaging modalities the light propagation in the biological medium or tissue varies distinctively [6]. Interaction between light and its respective biological medium or tissue provides information based on optical properties of the medium such as absorption coefficient, scattering coefficient and refractive index mismatch [1, 7]. The aforementioned information was crucial in optical imaging and benefits various optical imaging modalities. For example, in photoacoustic (PA) imaging, it is represented by varying absorbance in the medium. Optical coherence tomography (OCT), is an representation of the difference in elastic scattering coefficient of the medium.[8, 9]. And, Raman imaging exploits the inelastic scattering of photons [10, 11].

Numerical simulations were designed for light propagation in tissue for various imaging techniques [12-14]. Scattering of photons is theoretically determined by Rayleigh theory or Mie theory [15-17]. However, the limitation of these formulations was the inability of these to deal with mediums of significant absorption and scattering properties. In order to obtain an accurate image, it is often desired to have a good estimate of the photon distribution inside the tissue. Hence, a Monte Carlo (MC) simulation model was sought to investigate the photon propagation in tissue. Modeling using MC methods has long been considered the gold standard for predicting photon propagation in biological media [18]. Numerous MC codes have been developed to simulate diffuse reflectance and fluorescence from layered biological tissues, but little work has been done in this area with respect to Raman scattering.

MC modeling, was introduced by Wilson *et al.*, is a popular statistical computational algorithms method that depends on repetitive random sampling for studying light propagation in tissue [19]. Ultimately, the focus of MC modeling of light transport in multi layered tissue (MCML) users was to increase its efficiency [20]. With MCML written in standard C, it was used, continuously improvised and advanced. It has been modified to predict optical properties and study optical

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parameters such as transmission, absorption and reflectance [13, 21, 22]. Moreover, it has been further modified for other imaging techniques such as Raman imaging [23-25]. Here, in this study, MCML code was modified to handle embedded object and Raman photon generation.

Figure 1. Flow chart of Raman Monte Carlo with embedded object. s is the dimensionless step-size, ξ is the random number and d_b is the distance to the boundary.

2. METHODS AND MATERIALS

MCML written in standard ANSI C, propagates photons for a multi-layered medium (Fig. 1). Monte Carlo simulation uses three types of coordinate systems concurrently. They are Cartesian coordinate system, cylindrical coordinate system and spherical coordinate system. Firstly, a Cartesian coordinate system is used to trace photon packets, with origin as the point on the surface where the photon first enters the tissue surface. Secondly, a cylindrical coordinate system is used to score internal photon absorption. The cylindrical coordinate system is also used for the diffuse reflectance and total transmittance. They are recorded on tissue surface. Lastly, a spherical coordinate system, is used for sampling of the

propagation direction change of a photon packet. MCML code was modified to incorporate sphere, cylinder and ellipsoid [26]. At every scattering site distance between the current location of the photon and the object boundary is calculated. If the step-size taken by the photon is larger than the calculated distance then the photon is moved to the object boundary. At the boundary, based on Fresnel's law, the photon moves inside the objects or gets reflected back to the medium. Reflection or transmission of the photon depends on the angle of incidence of the photon with the surface of the object.

Figure 2. Simulation geometries. (a) layered medium, (b) embedded sphere, (c) embedded cylinder and (d) ellipsoid.

When light encounters molecules in the air, the predominant mode of scattering is elastic scattering, called Rayleigh scattering. In addition to elastically scattered light, a very small fraction of the incident light can also be scattered inelastically by processes such as Raman scattering, which involve energy transfer to or from internal excitations of the medium. Raman scattering has a low probability with only 1 in 10 million photons being scattered for most biologically relevant molecules [27].

MC has been improvised by incorporating Raman scattering to enable simulation of Raman imaging [28]. In reality, there is an elastic scattering at every scattering site. Therefore, for computational efficiency a normal scattering photon is converted to Raman photon at a predetermined Raman probability. The flowchart also highlights the tracking of the Raman photon in the medium using Monte Carlo simulation.

The layer was modelled to mimic human breast tissue [Fig. 2(a)]. A sphere of radius 2 mm was located at the depth of 3 mm whose optical properties mimic a tumor [Fig. 2(b)]. Cylinder was also assigned the optical properties of tumor. Cylinder was aligned with the x-axis and it extended to infinity along y-axis [Fig. 2(c)]. It was also located at the depth of 3 mm. Ellipsoid was also simulated with the optical properties of tumor. The ellipsoid was of 3 mm diameter along x-axis and 2 mm diameter along y-axis and z-axis was located at depth of 3 mm. Pencil beam from origin was used to illuminate the medium. Raman probability of 10^{-5} and 10^{-6} was simulated because the results of 10^{-6} for embedded object was very low [29]. On an event of Raman photon generation, the event's three-dimensional location is updated with the weight of the generated Raman photon.

3. RESULTS AND DISCUSSION

Raman – MCEO simulations were executed for 10^9 photons for both the Raman probabilities (RP). Grid size along z-axis is 500 μm . RP 10^{-5} took 12 hours, whereas simulation of RP 10^{-6} took 16 hours. It was observed that the signal from RP 10^{-5} was similar to that of 10^{-6} [Fig. 3(a)]. A-line scans of sphere, cylinder and ellipsoid was also observed prior to 2-D simulation [Fig. 3(b)]. It was possible to identify the presence of an object in the A-line scans, but the structural information was not available. Graph nature of both the Raman probabilities remain similar. This study also validates that one can run simulations of RP 10^{-5} . Simulations are yet to be executed to validate higher RPs. To illustrate the feasibility of 2D Raman simulation or B-scan, sphere [Figs. 4(a and b)] and cylinder [Figs. 4(c and d)] models were executed at 10^{-5} and 10^{-6} RPs. Sphere model took 22 and 24 hours. Cylinder model took 18-20 hours. B-scans of RP 10^{-5} , has strong signal from object which enables the boundary visualization.

Figure 3. Raman photon generated along the depth of the simulation mediums at Raman probability of 10^{-5} and 10^{-6} . (a) Layer, (b) sphere, cylinder and ellipsoid.

4. CONCLUSION

In this study, forward applications have been implemented whereby Raman techniques has been integrated with embedded objects. The modified simulation has been programmed to handle boundary conditions of the object. It is possible to provide useful information such as the diffused reflected, diffused transmitted, and absorbed Raman photons within the tissue with better accuracy compared to layered modelling [30]. Moreover, good simulation results were obtained and has provided useful predictions about the effect of tissue geometry. This was shown from the three shapes that exhibited clear B-scan images. However, in reality, breast tumors do not have planar boundaries with layers of normal tissue and are not infinitely broad and wide as what was carried out in this study. Nonetheless, modeling a layer of specific tissue based on its optical properties and embedding various simulation geometries are a reasonable first step in investigating the detection of small tumor projections.

On the other hand, modelling of Raman photons is not the physical representative of the Raman scattering. This is because in reality it is subjected to elastic scattering at every scattering site. Nonetheless, for computational efficiency, converting a normal scattering photon to Raman photon at a predetermined Raman probability is a best representation yet. It is also suggested to generate a Raman photon at a probability of 10^{-6} times the weight of the photon at every scattering site for improved results [25]. Additionally, number of photons greater than 10^9 would be sufficient to obtain significant output parameters. The major drawback of running adequate number of photons and probability would increase the computational expense. This drawback precludes this method from being used in applications where computation speed is important or when the result is required in real time, like in tissue spectroscopy.

In future work, improved importance sampling of Raman Monte Carlo simulations for tissue with embedded objects can be implemented to improve and to accelerate the performance speed. In MCML weight dropped by the photons is computed at every scattering site and photon drops weight in its path of travel. Hence, for computation efficiency, MCML can be further improvised through the study of step-size function of transport-length and weight drop.

Figure 4. B-scans of sphere (a-b), cylinder (c-d) and ellipsoid (e-f) for Raman probability 10^{-5} and 10^{-6}

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