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Monte Carlo Simulation of photons in biological tissues

The Monte Carlo simulation of photons in biological tissues begins by introducing a photon packet with a weight of w = 1. The photon packet is projected orthogonally at the interface where the position of the photon in the simulation is set at (x=0, y=0, z=0) in the <μ_x=0, μ_y=0, μ_z=1> direction. The interface or tissue surface is distinguished by a difference in the refractive indices which have influence over the transmissive and reflective properties of photons entering the tissue layer. In this case, the weight of the photon packet is reduced, thus setting the initial photon weight according the provided equation below into the simulation. In this simulation, the incident layer is n_1 = 1 while the tissue layer has a refractive index of n_2=1.37.

$$Entering\ weight = 1 - R_{sp} = 1 - \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} = \frac{0.37^2}{2.37^2} = 1 - 0.02437 = 0.9756$$

In addition, the angle of photon projection into the interface can also affect the transmission and the direction of entering photons. This transmissive and angle of propagation into the tissue is defined by Fresnel's equation. When the direction into the interface is not orthogonal, the photon weight and direction is updated as follow, where α_i and α_t are the incident angle and transmission angle respectively.

$$Entering\ weight = 1 - R_{sp} = 1 - 0.5 * \left[\frac{sin^2(\alpha_i - \alpha_t)}{sin^2(\alpha_i + \alpha_t)} + \frac{tan^2(\alpha_i - \alpha_t)}{tan^2(\alpha_i + \alpha_t)}\right]$$

In the simulation, the incident angle varies depending on the user input, while the transmission angle is dependent of the incident angle and can be calculated using Snell's law.

$$n_1 \sin(\alpha_i) = n_2 \sin(\alpha_t)$$

The entering photon direction is defined using equation 3.34 in the MCML paper.

$$\mu_x = \mu_x \frac{n_i}{n_t}$$

$$\mu_y = \mu_y \frac{n_i}{n_t}$$

$$\mu_z = \mu_z\, SIGN(\mu_z) \cos(\alpha_i)$$

All of this above sets the launch photon step of the simulation.

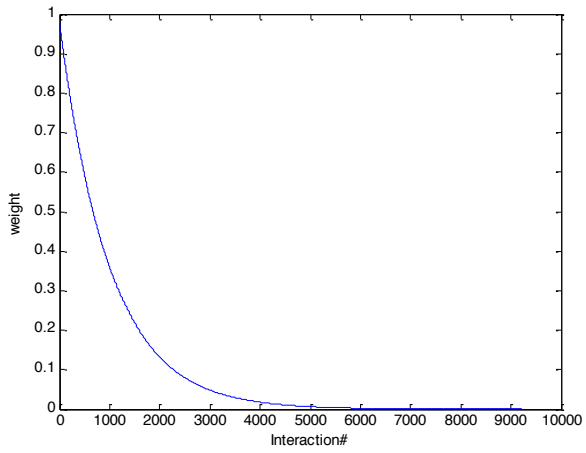
Subsequently, the photon mean path length is determined by a random dependent variable using the following equation. This is the distance at which a photon travels before hitting an interaction site.

$$s = \frac{-\ln(rand())}{\mu_t}$$

After interaction, the photon undergoes absorption where the weight is reduced accordingly after every photon movement in the simulation.

$$w' = w - \frac{\mu_a}{\mu_t} w = w - dw$$

Here, dw is the amount of photon weight being absorbed into the tissue during that interaction event. This value is recorded after every iteration in the simulation to determine the depth resolved absorbance or fluence of the tissue. Below is a plot of the photon packet weight after each iteration. For an orthogonal propagated direction, note that the initial weight is already reduced from the loss of tissue to air interface (w_i = 0.9756).



After absorption, the scattering of the photon is re-determined. The scattering is determined based on Henyey-Greenstein function which determines the cosine of the deflection angle, θ, and the azimuthal angle, φ.

$$cos\theta = \frac{1}{2g}\left\{1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g * rand()}\right]^2\right\} \; if \; g \neq 0$$

The value g measures the anisotropic scattering property of photons. In a typical tissue and for this simulation, this value is set to g = 0.9. Meanwhile the azimuthal angle is as follow.

$$\varphi = 2\pi * rand()$$

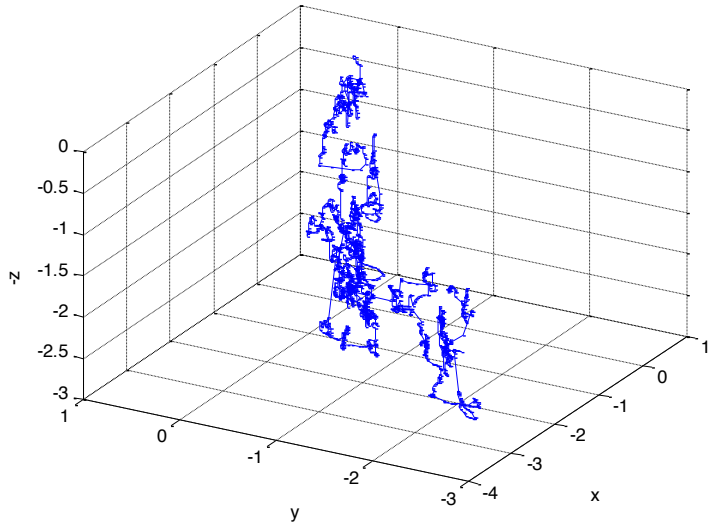
Knowing the deflection and azimuthal angle, the new photon direction, <μ_x, μ_y, μ_z> is updated using equation 3.24 provided in the MCML paper. Additionally, in a case where the previous direction is close to z axis (μ_z is near 1), equation 3.25 is used instead in the simulation.

In the case where the photon leaves the tissue or when the moving position of the photon is z<0, the direction and weight of the photon is recalculated based on the Fresnel's equation provided previously. However, the important consideration here in the simulation is the reflected photon. This photon goes through a weight reduction and due to the interface interaction and a change in direction (μ_z' = -μ_z) and position (z-axis) due to the reflection of the photon. This part of the simulation is outlined in section 3.8 of the MCML paper.

Following scattering, a weight checking algorithm is performed to measure the remaining weight of the photon and ensure whether the photon is either alive or dead. When a photon packet's weight falls below

the threshold of w < 0.0001, the new weight value goes through the Russian Roulette technique described in section 3.9 of the MCML paper. This technique uses a random (rand()) variable to determine the chance of an electron being about the survive. According to equation 3.36, the probability of a photon (that has a weight below the threshold) surviving is 1/m. In this simulation, m is set to 10. The purpose of this technique is to ensure photon weight conservation.

After the dead/alive determining step, the simulation finishes the iteration for 1 photon and keeps on going until the weight is determined dead (i.e. w = 0) by the Russian Roulette technique. When the photon is dead, the simulation exits the iteration and enters another iteration that simulates the next photon. A sample simulation of the propagating photon is visualized below, where the photon enters from above at position (0,0,0).

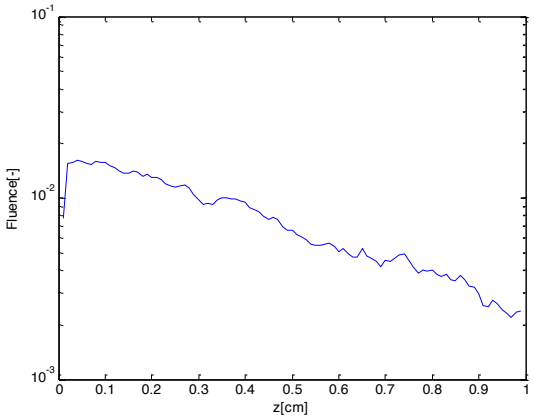


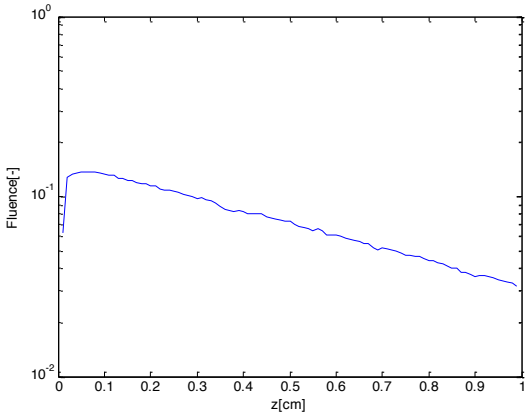
To solve for the depth resolved absorbance or fluence of the tissue, the photon weight (as described previously) is recorded after going through each absorbance. The weight absorbed value, dw, is updated to an array of the corresponding grid sized z position. The values are summed accordingly for every photons being simulated in the monte carlo simulation. The absorbance value is a direct sum of the dw, with respect to the z-axis. To convert to fluence, this can be done simply as follow.

$$Fluence(i_z) = \frac{A_z[i_z]}{\mu_a}$$

The result for depth resolved simulation of photons through a layer of tissue is shown below below, with parameters n = 1.37, g = 0.9, μ_a = 10 cm^{-1}, μ_s = 100 cm^{-1}, μ_t = 110 cm^{-1}.

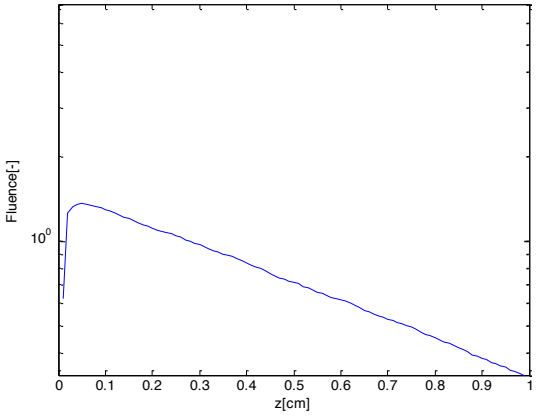
N = 100 N = 1000

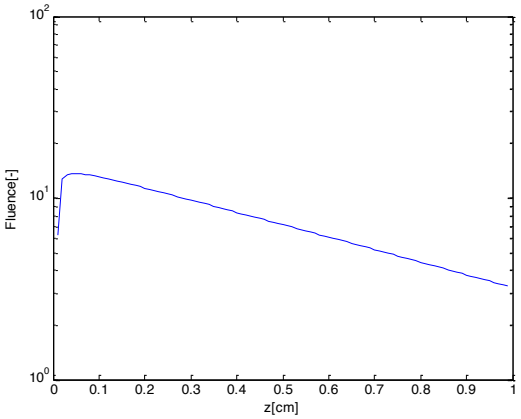




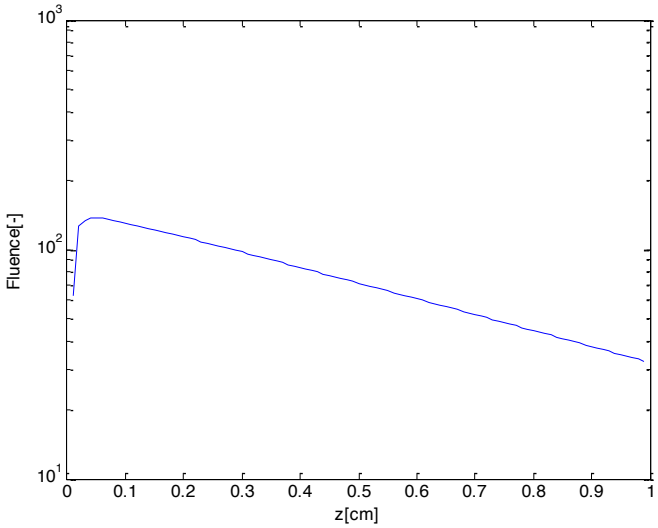
N = 10000

N = 100000





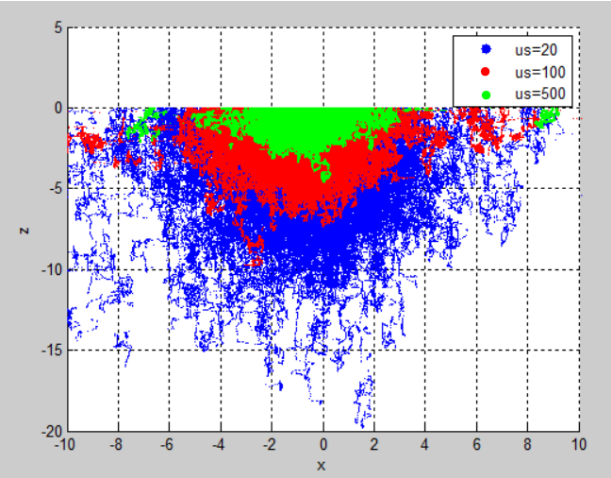
N = 1 million

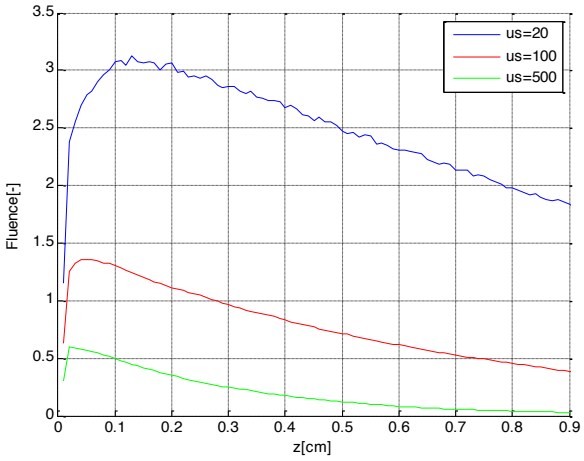


From these results, the sum of the absorbance value reduces the variations of the depth dependent fluence as more photons are being simulation. Comparing N = 100 with N = million, the fluence curve is a lot smoother with higher number of photons simulated. At the interface, where z = 0, the fluence is lower initially compared to z = 0.1 due to the internal reflection with the refractive differences or mismatch at the

interface. As z increases, or at higher depths into the tissue, the fluence decreases due to the decreasing weight of the photon packet as photons interact after each interaction. The estimated penetration depth is estimated to be around 0.6 cm.

The next goal is to visualize the photon propagation under different conditions in the Monte Carlo simulation. The parameters used were the same as previous runs except the scattering coefficient. Initially, the scattering coefficient was set at us=100. Therefore, to investigate the effect of scattering coefficient on the transport of photons, the coefficient is observed at us = 20,100, and 500 respectively. Below (left figure) is a visualization of photons propagating through air (n=1) into a tissue sample (n=1.37). Each point in the figure marks the position where the photon has traveled, marking the range of which light is deposited. In comparison, samples with higher scattering coefficient values have a higher frequency of scattering, thus loses photon packet much sooner. The result, shown for us=500, shows a smaller region of photon deposition as photons were do not travel very far when compared to samples with lower scattering coefficient. Samples with us=20 on the other hand, have the widest range of deposition. The is confirmed by the flounce measurement comparing the three scattering coefficient, shown below on the right. The figure is simulated using 10000 photons. From this figure, the lower scattering coefficient has a higher accumulation of photo deposition.





The transmission and the angle of transmission into the next layer (from air n=1 to tissue n=1.37) is guided by Snell's law and Fresnel's equation. In the simulation, the incident angle varies depending on the user input, while the transmission angle is dependent of the incident angle and can be calculated using the following equation. Here, 20°, 45°, and 70° are used respectively for comparison.

$$n_1 \sin(\alpha_i) = n_2 \sin(\alpha_t)$$

The amount of light entering through a boundary is defined by Fresnel's equation. When the direction into the interface is not orthogonal, i.e. pencil beam, the photon weight and direction is updated as follow, where α_i and α_t are the incident angle and transmission angle which is calculated from Snell's law.

$$Entering\ weight = 1 - R_{sp} = 1 - 0.5 * \left[\frac{sin^2(\alpha_i - \alpha_t)}{sin^2(\alpha_i + \alpha_t)} + \frac{tan^2(\alpha_i - \alpha_t)}{tan^2(\alpha_i + \alpha_t)}\right]$$

The parameters calculated for incident angles 20°, 45°, and 70° are shown in the table below.

Incident Angle (α_i)	Refracted Angle (α_t)	Reflected Intensity (Rsp)	Transmitted Intensity (w)	Direction ux	Direction uz
20°	14.46 °	0.0246	0.9754	0.24965	0.96834
45°	31.07 °	0.0326	0.9674	0.51614	0.85650
70°	43.31 °	0.1431	0.8569	0.68591	0.72769

From the calculation, it is shown that the higher the angle, more light is reflected, thus less light is transmitted into the tissue sample. Alternatively, the direction of the photon entering the tissue is changed. Below is a figure showing the photon deposition field and the fluence or accumulation of photon deposition across the z axis of the tissue. Using the same parameters for all simulations except for the angle of incident, lower angle yields slightly higher deposition at the interface due to the higher amount of light beam entering. From the fluence figure, the difference is noticeable when the incident angle is high, i.e. theta=70. However, the result from the visualization does not vary much as the light propagation behavior is similar in all three tissues within the simulation.