Biomedical Optical Spectroscopy and Imaging
Final Report for the Project

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Monte Carlo Simulation in Semi-Infinite Homogeneous Tissue

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Introduction:

The aim of the project is to run a simulation for 'N' (10 million) number of photons to calculate the following:

a) The total Reflected Fluence over an area of a radius of 5 cm around the origin.
b) The spatially resolved reflectance and then to fit the continuous wave semi-infinite solution of the photon-diffusion equation, in order to estimate the μ_{eff}. Also, to compare the calculated μ_{eff} to the estimated μ_{eff} from the fitted curve.
c) The time-resolved photon reflectance at source-detector separations of ρ = 1 cm, and ρ =2.5 cm. And to plot (histogram) the arrival of photons as a function of time in second.

Monte Carlo Simulation:
Monte Carlo simulations are used to model the probability of different outcomes of a process that cannot be easily predicted due to the intervention of random variables.
A novel simulation method of Monte Carlo is used to predict the photon propagation path that takes during its journey within the tissue.
Here, it is assumed that Monte Carlo simulations of photon propagation or transport are in semi-infinite and homogeneous tissues. These two assumptions are made to simplify the problem. By considering the tissue to be semi-infinite it is no longer needed to calculate transmission of photons (T=0) and by considering the homogeneity of the tissue it is not needed to update the tissue optical properties μ_a and μ_s for different tissue layers.
In the simulation, random numbers are generated to simulate probabilistic events. The random numbers are used to sample the known probability distribution that describes each interaction of the photon with tissue.

$$\int_a^b p(x)dx = 1$$

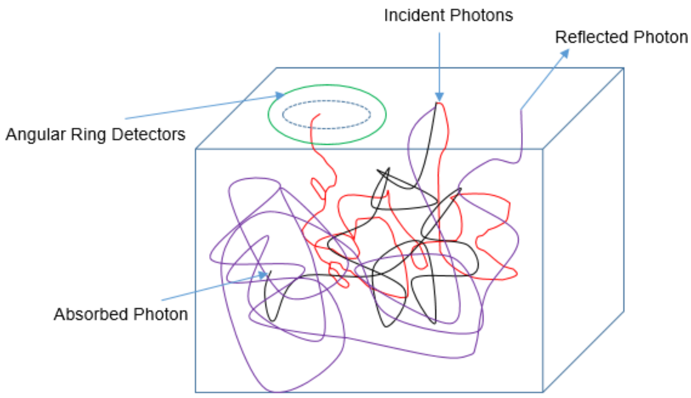


Fig. 1. Photon transport in a semi-infinite tissue of homogeneous quality

Methods:

Using the Monte Carlo method, the photon propagation within the tissue can be computed. These propagation steps are expressed as probability distributions, which describe the step size of the photon movements. The photon can have mainly three fates. It can get absorbed, transmitted or reflected. In this project, there will be no transmission because the tissue has been considered to be semi-infinite. Therefore, only the absorption and the reflection of the photons are considered for calculation of the photon transition with the tissue.
The process of calculating the reflection and absorption as done in the (*MonteCarlo.m)* Matlab code is described step by step in the subsequent report.
To account for the Specular Reflection, the following is calculated:

$$Specular\ Reflection = \frac{(\text{nout} - \ \text{ntissue})^2}{(\text{nout} + \ \text{ntissue})^2}$$

where,
nout = refractive index of the air.
ntissue = refractive index of the tissue.
Specular reflection is the reflection that occurs in the surface of the tissue because of the difference in refractive index of air and tissue. This will result in the reduction of the photon weight w= 1- specular weight.

First, the photon step size is calculated using the following formula and the coordinates of the photon i.e. the x, y, and z are updated.

$$\mathbf{s_1} = -\frac{\mathbf{log(\zeta)}}{\boldsymbol{\mu_s}}$$

$$\mathbf{x'} = \mathbf{x} + \boldsymbol{\mu_x}\mathbf{s_1}$$
$$\mathbf{y'} = \mathbf{y} + \boldsymbol{\mu_y}\mathbf{s_1}$$
$$\mathbf{z'} = \mathbf{z} + \boldsymbol{\mu_z}\mathbf{s_1}$$

The absorbed weight is then calculated and added to the absorption matrix of the photon.

$$\textbf{Weight absorbed} = \textbf{weight of photon} \times \frac{\boldsymbol{\mu_a}}{\boldsymbol{\mu_t}}$$
$$\mathbf{A} = \mathbf{A} + \textbf{weight absorbed}$$

The weight of the photon is then updated by subtracting the absorbed weight from the original weight.

$$\textbf{New weight} = \textbf{original weight} - \textbf{weight Absorbed}$$

When a scattering event occurs angles of deflections in a photon's trajectory is calculated using the following formula. Where θ is the scattering angle, ϕ is the azimuthal angle and g is the anisotropy factor.

$$\boldsymbol{cos\theta} = \begin{cases} \frac{1}{2g}\left(1 + g^2 - \left[\frac{1-g^2}{1-g+2g\zeta}\right]^2\right) & g \neq 0 \\ 2\zeta - 1 & g = 0 \end{cases}$$

$$\boldsymbol{\phi = 2\pi\zeta}$$

The new direction cosines are then calculated based on the calculated values of $\theta\ and\ \phi$. If the $|\mu\_z|$ < 0.9999 then the following formulas are used.

$$\boldsymbol{\mu'_x = sin\theta \frac{\mu_x\mu_z cos\phi - \mu_y sin\phi}{\sqrt{(1-\mu_z^2)}} + \mu_x cos\theta}$$

$$\boldsymbol{\mu'_y = sin\theta \frac{\mu_y\mu_z cos\phi - \mu_x sin\phi}{\sqrt{(1-\mu_z^2)}} + \mu_y cos\theta}$$

$$\boldsymbol{\mu'_z = -sin\theta cos\phi\sqrt{(1-\mu_z^2)} + \mu_z cos\theta}$$

If μ_z > 0.9999 then following equations are used to update direction cosines.

$$\boldsymbol{\mu'_x = \sin\theta\ cos\phi}$$
$$\boldsymbol{\mu'_y = sin\theta\ sin\phi}$$
$$\boldsymbol{\mu'_z = SIGN\ (\mu_z) \cos\theta}$$

After the direction cosines are updated, the photon's fate of survival is checked by the following formula:

rand()<=(1/m)

If the photon weight is below the threshold that is set to epsilon=0.0001, then the photon enters a roulette and it has 1/m chance to survive where 'm' is 10. If the photon survives then the photon weight is updated or it will be set to zero because it is now no longer alive.

$$w = m * w$$
Or,
$$w = 0$$

The z coordinate value of the photon is checked to infer whether a photon is reflected or not. If the z coordinate is less than 0 then the photon is considered to be reflected. The z axis is the tissue and air horizon.

Solution to question 1:
The total reflected fluence over an area of a radius of 5 cm around the origin is required to be calculated.
By definition, the Fluence is the energy per unit area at position $\vec{r}$ integrated over all directions. Its units are J/cm^2.
Therefore, to calculate the reflectance only inside the circle of radius 5 cm, a condition is set to check if the photon's current position is inside the radius as given.

$$\textbf{Radius} = \sqrt{(\boldsymbol{x^2 + y^2})}$$

Where x and y are current x and y co-ordinates of the photon. If the photon position lies within the mentioned radius i.e. 5 cm, then the R_rho variable is updated that stores the reflectance value for that position.

Solution to question 2:
The spatially resolved reflectance is calculated and fitted to the continuous wave semi-infinite solution of the photon-diffusion equation, in order to estimate the μ_{eff}.
The reflectance is calculated within a ring of 20% width of a rho value (source detector separation) that is selected at 0.5 increment from 1 to 5 cm.
The ring of detection will be 10% on exterior and interior of the circumference with radius rho.

$\rho - d\rho \leq \rho_{exit} < \rho + dp$
Where $d\rho = 0.1 \times \rho$ and $\rho_{exit}^2 = x_{exit}^2 + y_{exit}^2$

For fitting, the ratio of the fluence (ϕ_{cw}) at the initial source-detector separation (rho=1 cm) to fluence at every other source-detector separation is used as the fitting curve.

$$\phi_{cw}(\rho_o = 1) = p_{cw} \frac{\left(3(\mu_s' + \mu_a)\right)}{4\pi} \exp\left(-\rho_o \sqrt{3\mu_a(\mu_a + \mu_s')}\right) * \frac{1}{\rho_o} \quad \text{------(1)}$$

$$\phi_{cw}(\rho) = p_{cw} \frac{\left(3(\mu_s' + \mu_a)\right)}{4\pi} \exp\left(-\rho \sqrt{3\mu_a(\mu_a + \mu_s')}\right) * \frac{1}{\rho} \quad \text{-----(2)}$$

Taking the ratio between (2) and (1):

$$\phi = \frac{\rho_o e^{-\mu_{eff} * \rho}}{\rho e^{-\mu_{eff} * \rho_o}}$$

Where,
$\phi(\vec{r}, t)$: Photon fluence rate in $\mathrm{W/cm^2}$
ρ : Source detector separation
ρ_o : Source detector separation at 1 cm
The μ_{eff} is given by $\mu_{eff} = \sqrt{3\mu_a(\mu_a + \mu_s')}$ in cm^{-1}

Solution to question 3:
The time-resolved photon reflectance at source-detector separations of ρ = 1 cm and ρ =2.5 cm are computed. The time-resolved photon reflectance is calculated by keeping track of the photon path length and then dividing it with the speed of light 3×10^{10} $cm/\sec^2$. Photons with longer path length will require more time to travel. The total path length (s) is given by $\sum i\ s_i$ where s_i is the step size. Therefore, we can conclude that photons that travel deeper into the tissue will have a higher value of time of flight.
The time of arrival of the photon is then $t_{arrival} = \frac{s}{v}$ which is the time of flight for that photon.
In the program the source detector separation is taken to be 1 cm and 2 cm and the time resolved photon reflectance is computed for each of the detector position with 10% bandwidth in both the interior and the exterior of the detector ring.
A vector is assigned to store the path length of each of the photon and then each path length of the photon is dived the speed of light to get the time of flight.

Flowchart for the Monte Carlo simulation:

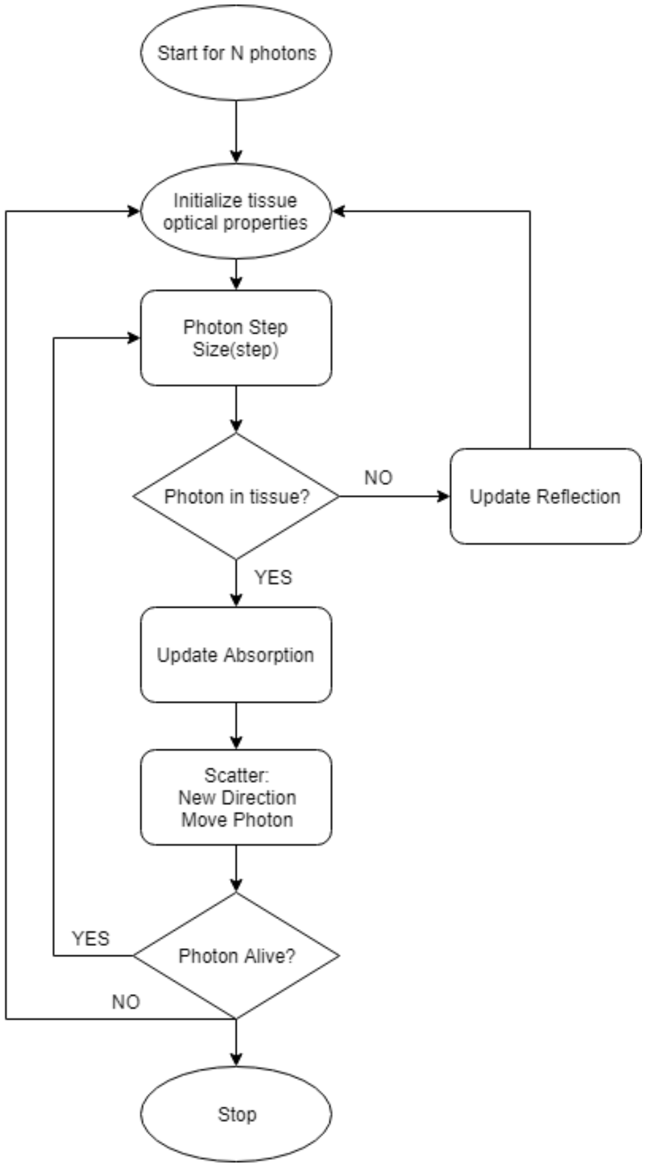


Fig 2: A flow chart for the Monte Carlo simulation in semi-infinite and homogeneous tissue.

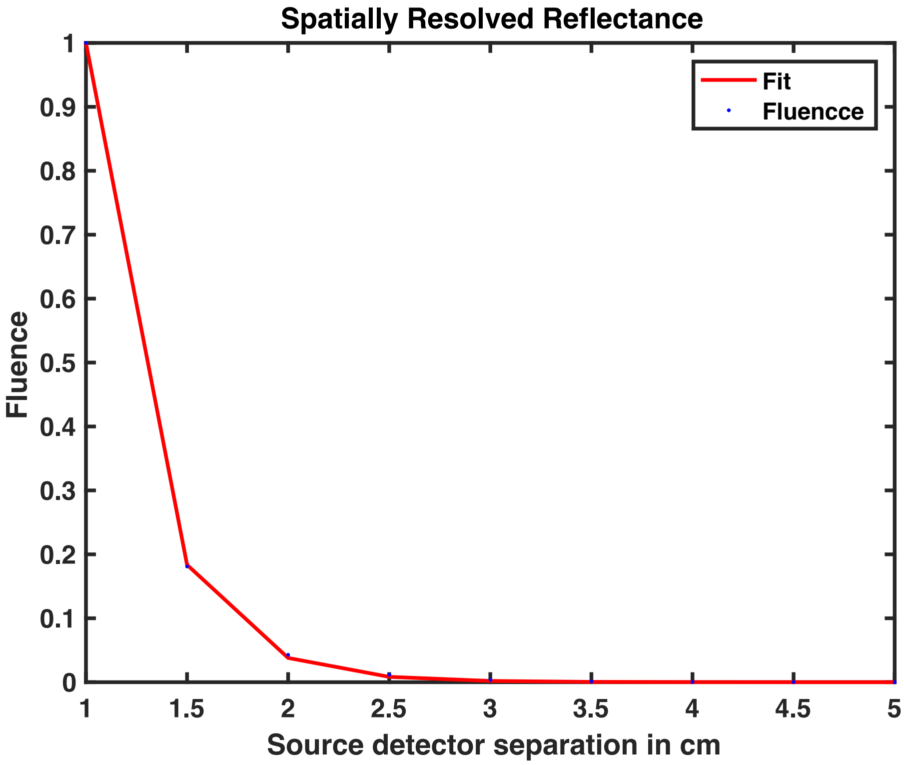
Results:

1. The Program was run for 10 million photons for a source-detector separation of 5 cm. The fluence over an area of radius 5 cm was $\frac{7.13 \times 10^\wedge 6}{area} J/cm^2$ where area = $\pi r^2 = 78.53\ cm^2$. Therefore, the fluence is $\mathbf{9.07 \times 10^4\ J/cm^2}$.

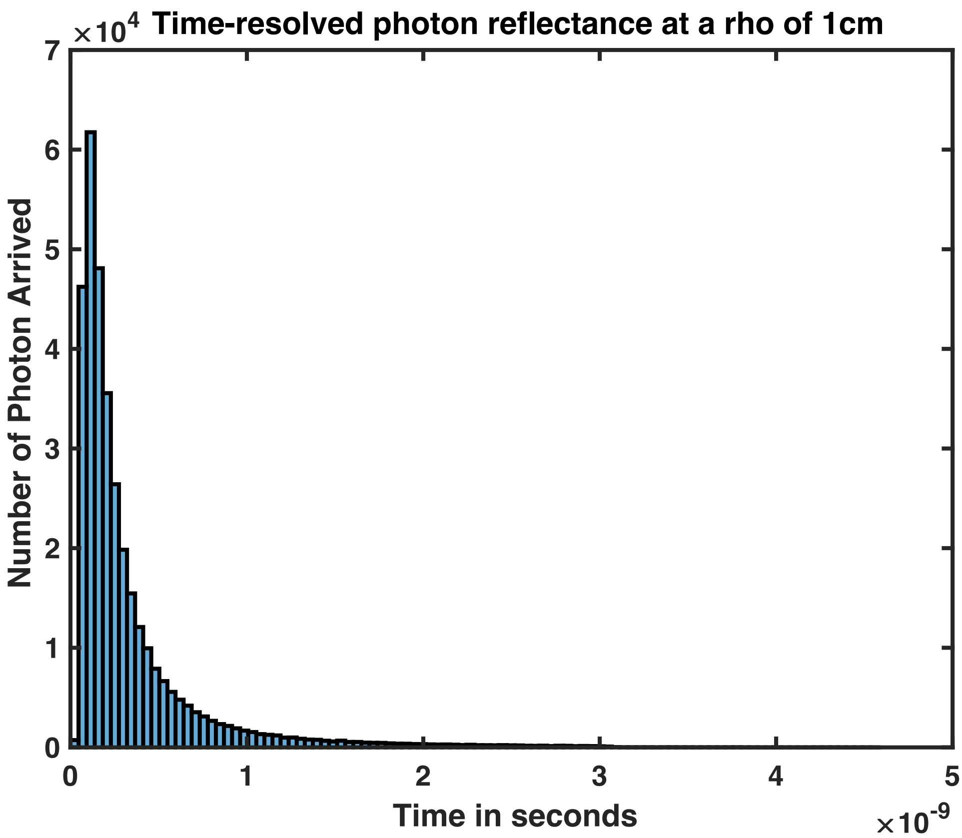
2. From the fitted curve the estimated μ_{eff} is **2.57cm^{-1}.** The μ_{eff} calculated is **1.65 cm^{-1}** from the equation $\mu_{eff} = \sqrt{3\mu_a(\mu_a + \mu_s')}$ in cm^{-1} $where\ \mu_a\ is\ 0.1\ \ cm^{-1} and\ \mu_s' = 9\ \ is\ \ \ cm^{-1}$.
The μ_s' was calculated using the following formula:
$\mu_s' = \ \mu_s(1 - g)$
$\mu_s = 100cm^{-1}$
$g = 0.91$

3. The time-resolved photon reflectance at source-detector separations of ρ = 1 cm and ρ =2.5 cm are computed. The histograms of the probable number of photons are plotted against time is seconds.
The peak value of the histogram for source detector separation 1 cm is 6.17×10^4.
The peak value of the histogram for source detector separation 2.5 cm is 4781.

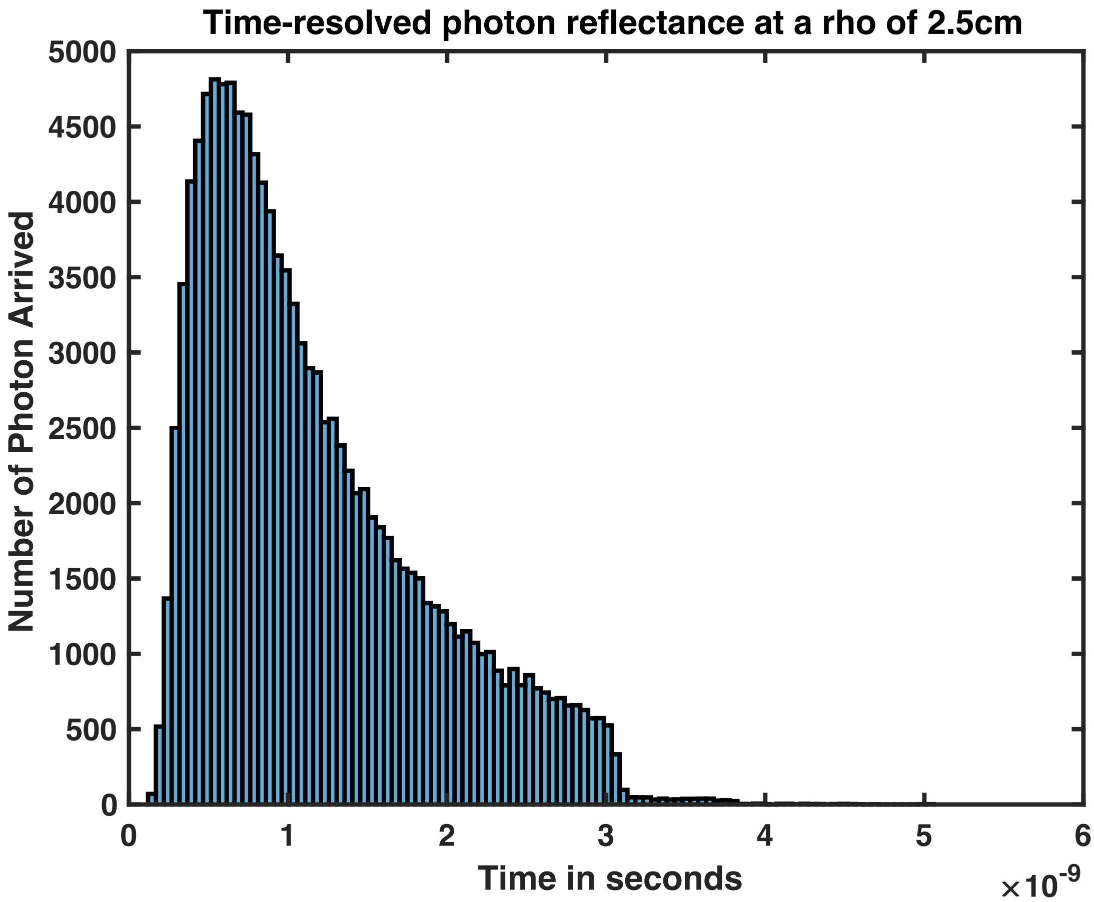
Result for Question 2:
The following is the graph of the Spatially resolved reflectance measured as a function of source-detector separation:



Result for Question 3:
The following is the histogram of the time resolved reflectance measured at source-detector separation of 1 cm:



Result for Question 3:
The following is the histogram of the time resolved reflectance measured at source-detector separation of 2.5 cm:



Discussion:

1. The total reflected fluence over an area of radius 5 cm was calculated but factors such as specular reflection, non homogeneity of the tissue or the tissue finitness was not considered.
2. For reasons of verification the estimated spatially resolved reflectance is fitted the to the continuous wave semi-infinite solution of the photon-diffusion equation. This fit helps to verify the data obtained by the monte carlo simulation.
The plot is of the normalized fluence instead of the raw fluence that is obtained. This normalization is done in order to have same range of values for each input. It will therefore make computing less sensitive to the scale of the variable.
The difference in the calculated and the estimated μ_{eff} is because of mainly two sources errors. Firstly, the difference can be greatly reduced by increasing the number of photons for which it is simulated. Moreover, the difference in refractive index between the air and the tissue medium is not considered, which will lead to some reflection of light inside the the tissue. This results in inaccurate calculation of reflection of light around the tissue surface.
The mean square error between the estimated and the calculated μ_{eff} is $2.57 - 1.65 = 0.92$.
3. The histogram of the number of photons arriving against time in seconds was plotted for two source detector separation 1 cm and 2.5 cm. But, the proper fit was not possible because of the dissimilarities in the simulated data to the calculated data. This dissimilarity may be accounted for the fact that the solution is for the time of flight of the photons but the histogram plots the number of photon.

References:

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4. *A primer on Monte Carlo simulation of light-tissue interaction* by Dr. Ashwin B Parthasarthy.
5. Light Transport in Tissue – Monte Carlo annotated by Dr. Ashwin B Parthasarthy.

Acknowledgment:

1. Ashwin Parthasarathy, Ph.D., Assistant Professor, University of South Florida.
2. Biomedical Optical Spectroscopy classmates.
3. Figure 1 is done in power point and Figure 2 is done in the https://www.draw.io/.
4. All results are obtained from matlab code MonteCarlo.m.