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DEPARTMENT OF PHYSICS

B.TECH PROJECT - EP 4275

Measuring Spectral Reflectance Using Photon Transport Monte-Carlo Multi-Layer Simulation

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1 Introduction

The interaction of light and tissue is a subject of much importance in Biomedical studies. When a photon propagates through tissue it interacts with the various layers of skin in different manners, depending on the layer parameters. The main processes are absorption and scattering. The problem posed here is of analysing the response of the tissue and its constituents, to the spectra of light; in the form of its reflectance. The analytical solution to this problem lies in solving the Radiation Transport Equation, with no emission. For a complex structure such as the skin's this is difficult, and thus a stochastic method is used. Here, we use a Monte-Carlo (MC) based simulation of a photon bunch, assuming a nine-layer model[1] of the skin and five defining parameters of each layer.

1.1 Layers

The skin is primarily divided into the epidermis, dermis, and the subcutaneous tissue. For our purposes we divide it into nine layers as indicated below.

1.2 Parameters

Each layer is defined along with the following parameters.

- Absorption Coefficient, μ_a
- Scattering Coefficient, μ_s
- Anisotropy Scattering Coefficient, g
  g is the average of the scattering coefficient of the cosine of the scattering angle. For a g 1, the medium is forward scattering, and the for g -1, it is backward scattering.
- Refractive Index, n
  Is used to calculate the photon trajectory at boundaries of the layers.
- Thickness, t

The attenuation coefficient

$$\mu_t = \mu_a + \mu_s \tag{1}$$

is used to decide the step-size of the photon in the MC simulation.

2 Method

The MC simulation attempts to send multiple photons in the layered-tissue and measure the fraction of photons reflected back through the top layer of the skin. However, a photon-by-photon simulation would resource-intensive and laborious. Instead, a photon bunch is assumed with a unit weight to start. Each interaction results in a loss of weight and that

weight is consequently added to the absorption, reflection, or transmission count of photons. The following steps are used to simulate about 10,000 photon bunches for wavelengths in the visible light range (350-750 nm)[2].

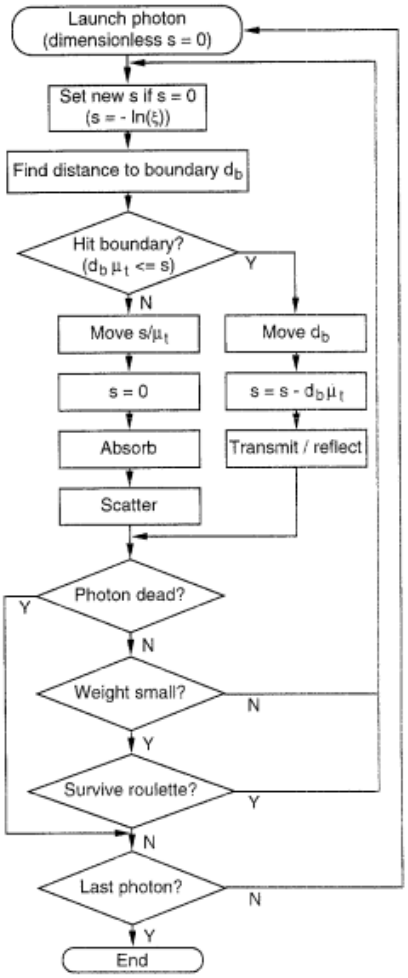

Figure 1: Flowchart Showing The Method Used [2]

2.1 Step 0 - The Set-up

The layers along with their parameters are defined. The photon bunch is initialised with a zero position vector and a z-direction unit vector for propagation.

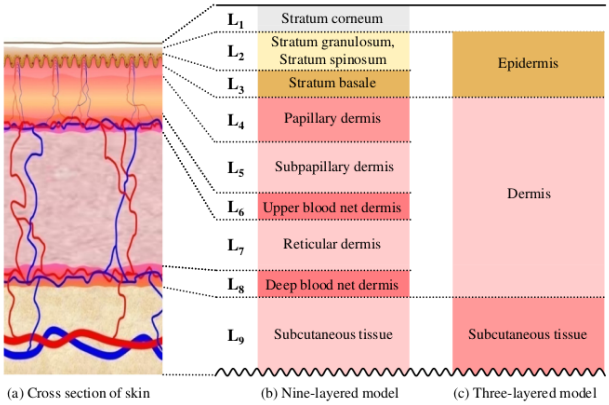

Figure 2: Nine-Layered Model[1]

2.2 Step 1 - Photon Incidence and Step-Size

A photon of unit weight strikes the first layer with normal incidence. Here, the photon may experience specular-reflectance and some weight may be deducted.

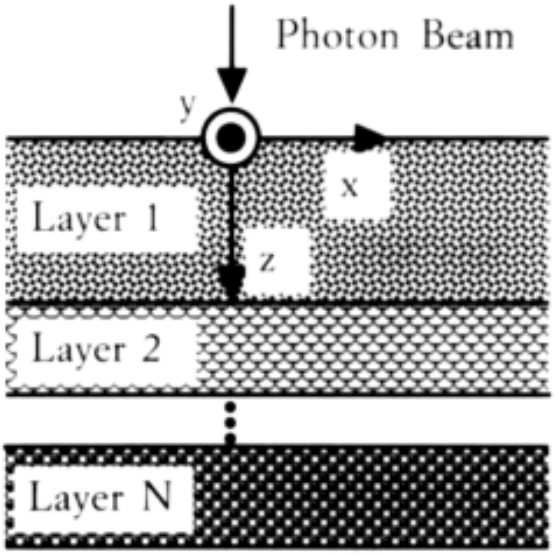

Figure 3: Initial Photon Launch[2]

Once inside the medium, a step-size for the photon is decided based on the Mean-Free-Path obtained from the definition of the attenuation coefficient (μ_t) and a random number $\zeta \in (0.0, 1.0)$

$$s = -\frac{ln(\zeta)}{\mu_t} \quad s \in (0.0, \text{inf}) \tag{2}$$

As seen in the equation above, the step-size may over-step the current layer of photon. In this case, the photon is moved to the next boundary and:

$$s_1 = s - d_b \mu_t \tag{3}$$

2.3 Step 2 - Transmission/Scattering and Absorption

After the photon has been moved using its direction cosines, its fate is decided, depending on whether it is at the boundary of two layers or inside the medium.

1. If at the boundary, using the reflectance formula, and a random number, it is decided whether the photon will be reflected back or transmitted.

2. In the other case, it undergoes absorption by deducting a proportionate weight. Scattering is decided using the Henvey-Green scattering function.

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

The direction cosines are updated thus, for either transmission, internal reflection, or scattering.

2.4 Step 4 - Death

The photon's simulation/lifetime can come to end in two ways:

1. Transmission - The photon escapes into the ambient medium either through the first or last layers, thus being counted under the diffuse reflectance or transmittance.

2. Russian Roulette - To increase the speed of the simulation, the R.R scheme is employed, where if the photon's weight is below a threshold, it is subjected to an appropriate test to decide if it can be terminated, whilst also not aggressively violating the conservation of energy. The scheme is as below:

$$W \leftarrow \begin{cases} mW & \zeta \leq \frac{1}{m} \\ 0 & \zeta > \frac{1}{m} \end{cases}$$

2.5 Step 5 - Scoring Quantities

The three quantities of absorbance, reflectance, transmittance are scored as below:

1. Absorption, A - Wherever the photon undergoes absorption, the array for absorption at that wavelength is updated.

2. Diffuse Reflectance, R_d - When a photon exits the tissue through the first layer into the ambient medium, its weight is scored into the corresponding array.

3. Diffuse Transmittance, T_d - When a photon exits the tissue through the last layer into the ambient medium, its weight is scored into the corresponding array.

The final values are calculated by dividing the sum of the array values by the number of photons.

3 Code

The code, along with the graphs and results from this report, is available here - Github - SkinSim

4 Optimizing Parameters

Following the reference, the different absorption, scattering, and anisotropy coefficients need to be initialised for the nine-layer model.

4.1 Absorption Coefficients

The Stratum Corneum's (L1) is based on a baseline amount of skin absorption.

$$\mu_{a,sb} = 0.244 + 85.3exp\left[-\frac{\lambda[nm]-154}{66.2}\right](cm^{-1})$$

For the epidermis (Layer 2 and 3), the coefficient is based on baseline skin and melanin absorption:

$$\mu_{a,e}(\lambda) = C_m\mu_{a,m}(\lambda) + (1-C_m)\mu_{a,sb}(\lambda) \quad (cm^{-1})$$

$$\mu_{a,m}(\lambda) = (6.6\times10^{11}).\lambda[nm]^{-3.33} \quad (cm^{-1})$$

L3's coefficient is weighted with a parameter k_{mel}, for which a value is chosen to optimize results.

$$[\mu_{a,e}(\lambda) \text{ for } L_2] = k_{mel}.[\mu_{a,e}(\lambda) \text{ for } L_3]$$

For the Layers 4-9 (dermis and subcutaneous) absorption is determined through the haemoglobin concentration, using the whole-blood concentration(C_b) and its absorption coefficient($\mu_{a,b}$)

$$\mu_{a,d}(\lambda) = C_b\mu_{a,b}(\lambda) \quad (cm^{-1})$$

$$\mu_{a,b}(\lambda) = 2.303\times\frac{G}{W}\times\varepsilon_{hb}(\lambda) \quad (cm^{-1})$$

$$\varepsilon_{hb}(\lambda) = SaO_2.\varepsilon_{oxy}(\lambda) + (1-SaO_2).\varepsilon_{deoxy}(\lambda)$$

ε_{hb} is the molar extinction coefficient of haemoglobin. The values are drawn from the curves provided in the reference with SaO_2 (oxygen saturation) as 80%. The haemoglobin concentration(G) and its gram molecular weight(W) are taken as 150 and 64,000 respectively. The absorption factors for L4-L9 are set with weighting factors.

$$[\mu_a(\lambda) \text{ for L4-L9}] = k_b.\mu_{a,b}(\lambda)$$

The factors are obtained from the graph referenced in the paper.

Table 1: Factors For Absorption Coefficients

Layer	k
L1	-
L2	0.23
L3	-
L4	0.0445
L5	0.0445
L6	0.3212
L7	0.0445
L8	0.1076
L9	0.05496

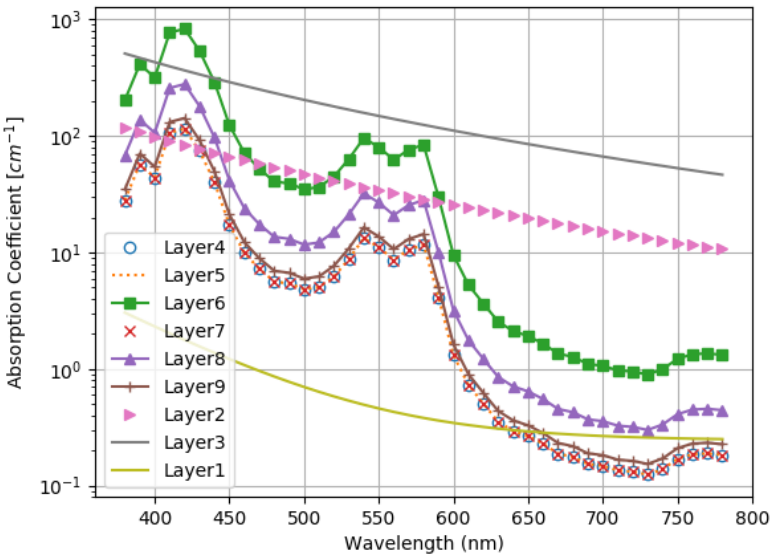

Figure 4: Absorption Coefficients

4.2 Scattering Coefficients

The scattering coefficients for the epidermis and dermis are given by the combined effect of Rayleigh and Mie scattering.

$$\mu_{s,s}(\lambda) = \frac{\mu_{s,R}(\lambda) + \mu_{s,M}(\lambda)}{1-g}$$

$$\mu_{s,R} = (2 \times 10^{12})\lambda\ [nm]^{-4} \quad (cm^{-1})$$

$$\mu_{s,M} = (2 \times 10^{5})\lambda\ [nm]^{-1.5} \quad (cm^{-1})$$

Each layer has to be multiplied by a factor k_s to optimize the results.

$$[\mu_s(\lambda) \text{ for L1-L8}] = k_s.\mu_{s,s}(\lambda)$$

The μ_s for the last layer (L9) is given as below:

$$\mu_s(\lambda) = k_{s9} \times 527 \exp\left(-\frac{\lambda[nm]}{222}\right) + 99 \quad (cm^{-1})$$

Table 2: Factors For Scattering Coefficients

Layer	k
L1	1.5982
L2	0.7862
L3	0.8571
L4	0.6214
L5	1.0
L6	0.6547
L7	0.8452
L8	4.1667
L9	0.3

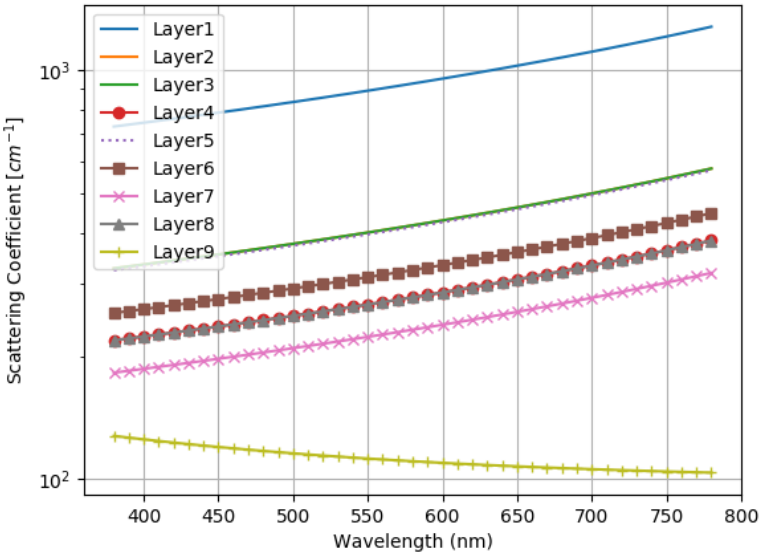

Figure 5: Scattering Coefficients

4.3 Anisotropy Coefficients

A layer-dependent g is not yet used, instead the following formula is employed:

$$g(\lambda) = 0.62 + (0.29 \times 10^{-3} \times \lambda[nm])$$

This needs to be changed to be layer-dependent.

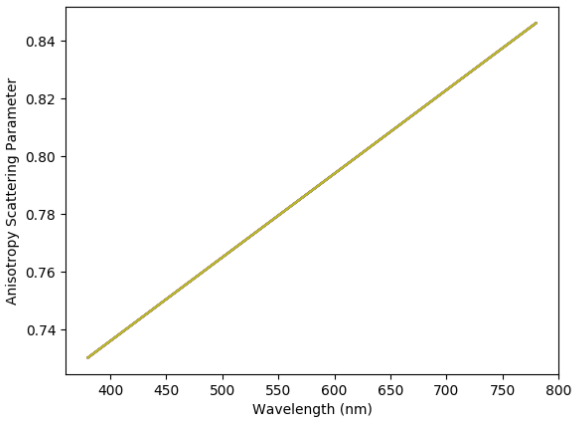

Figure 6: Anisotropy Coefficients

5 Results

Using the parameters mentioned above and their corresponding factors from observation, the following result is obtained, with reference to the data given in the results. 10,000 photon bunches were used to run the simulation, running for about 2 hours initially but shortened to 30-40 minutes after a little code optimization concerning the random number generation.

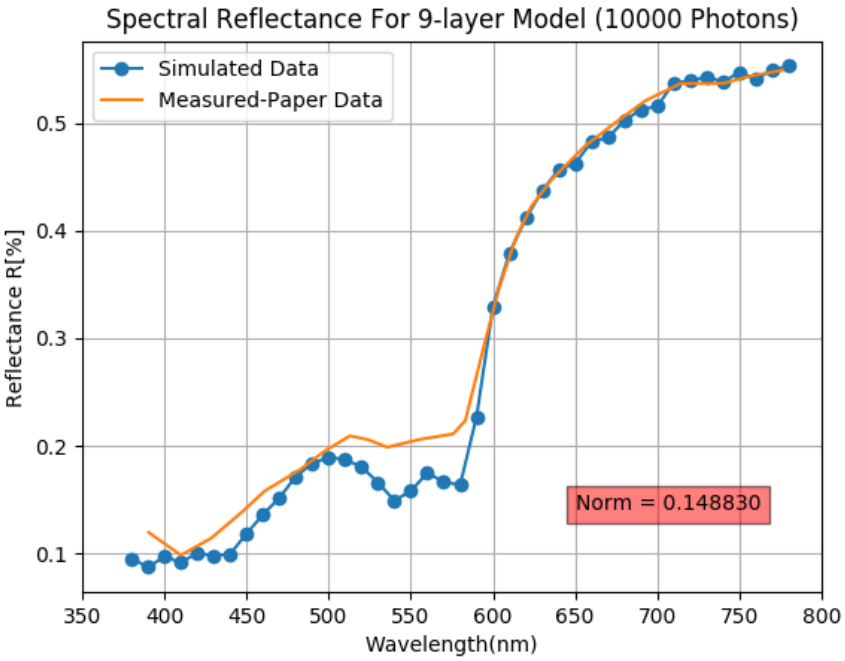

Figure 7: Spectral Reflectance results compared to measured data for a 27-year old man, C_m=0.30

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Total Weight (R+T+A):  1.0000003499660468
Mean Scatters:  311.0035
Mean Distance(cm):  0.19942246674638706
Time (minutes) 37.41786700089772
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Figure 8: Statistics From Simulation

6 Shortcomings and Errors

- The factors for absorption, scattering, need to be optimized. At the moment I have done this just by observing the change in the graph by changing parameters. I am not sure about what to do about this.
- The graph is not properly fitted to the measured data at lower wavelengths, most probably due to inexact absorption factors.
- The data for the parameters for the nine-layered model is vague, and needs to be studied better.

References

[1] Takaaki M AEDA et. al. Monte carlo simulation of spectral reflectance using a multilayered skin tissue model. 2010.

[2] Lihong Wang et. al. Mcml - monte carlo modeling of light transport in multi-layered tissue. 1995.