Biomedical Optics

Light Scattering in Tissue by Monte Carlo Simulation

E. Göran Salerud

IMT 2006-10-05

What is Monte Carlo Modeling?

Monte Carlo Modeling is a method that can be used to simulate photon interaction with tissue. The models can be built such that increasing complexity can be added as the model develops. Thus, the model develops from a simple concept of random number generation to a very accurate interpretation of photon propagation in tissue.

Program Menu

The steps that will be needed to implement a Monte Carlo model of photon propagation in tissue are listed below and are explained in the remainder of this presentation.

- Step 1: Random Number Generation
- Step 2: Attenuation of Collimated beam in Tissue
- Step 3: Scattering of Photons in Tissue
- Step 4: Anisotropic Tissue
- Step 5: Index Mismatch of Boundary Layers
- Step 6: Grid Structure
- Step 7: Finite Beam Width
- Step 8: Multiple Layers
- Step 9: Fluorescence
- Step 10: Detector

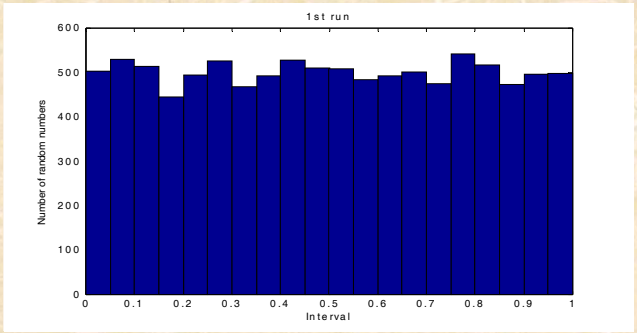
Step 1: Random Number Generation

- The first step in building a Monte Carlo model is to develop a method to create random numbers.
- Step 1 simply deals with creating a random number function generator. We use a uniform distribution of random numbers, which gives r.n. between 0 and 1.
- The p.d.f of a uniform distribution of r.n. is a constant 0.1 over the interval (0,1).

Step 1: Concepts

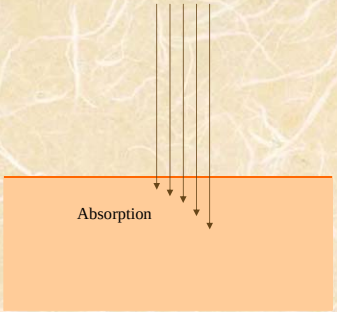
- This r.n. is "uniformly", i.e., equally distributed
- First, generate 10,000 r.n. and divide the (0,1) axis into 20 equal intervals.
- Observe the frequency of occurrence of r.n. in each interval. The ideal mean value is 500.
- Observe the standard deviation. The standard deviation should be less than 36.

Step 1: Results



Step 2: Attenuation of a Collimated Beam

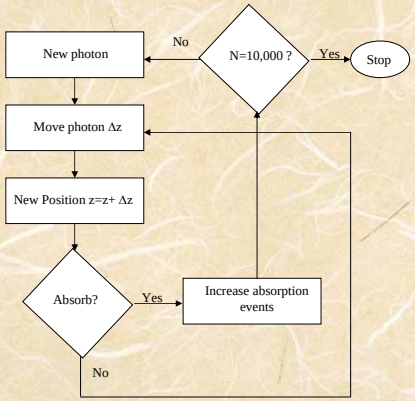
- The goal of this step is to figure out how photons are absorbed in tissue.
- Absorption coefficient is defined as μ_a with units cm^{-1}.
- The probability of absorption with the medium per unit path length in the interval $[s_1,\ s_1 + ds]$ is defined as $u_a ds_1$.
- Absorption is defined by Beer's Law: $E = E_o e^{-\mu_a x}$, where x is the depth of tissue.



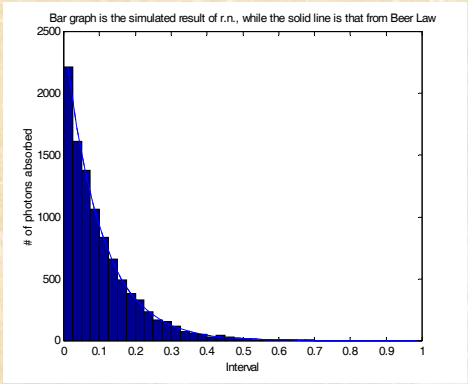
Step 2: Concepts

- After moving a step, a photon is either absorbed or scattered. However, to simplify the problem, we only consider absorption in this step, that is , no scattering occurs. Therefore, $\mu_t = \mu_a = 10\ cm^{-1}$ in this program.
- To simplify further, assume index matched boundary ($n_1 = n_2$), fixed step, and fixed weight photon.
- Index match means that no reflection occurs at the boundary.
- Fixed step means that absorption only happens at the end of a fixed step Δz. In this program, $\Delta z = 0.025$ cm.
- Fixed weight photon means that a photon is treated as an integral particle. A photon cannot be partially absorbed.

Step 2: Flow Chart

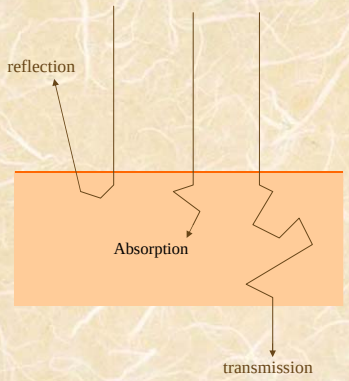


Step 2: Results



Step 3:
Scattering of Photons in Tissue

- In the third step scattering is incorporated into the model.
- Here photons will either be absorbed, transmitted through the tissue or reflected back from the tissue.
- We will keep track of each photon and tally where all the photons terminate.
- In this case, boundaries are index matched.
- The step length of each photon is variable.



Step 3: Concepts

- In this step we will simulate the scattering of a photon in tissue.
- Scattering is accomplished by accounting for the position and direction of each photon
- If a photon exits the tissue, it has been reflected or transmitted. Determining which depends on the z position at the exit point. Z < 0 means reflected and Z > tissue depth means transmitted. At this point the photon is terminated.
- Termination of the photon can also occur due to absorption in the tissue.
- Step length is no longer a fixed value. It is calculated as:

$$S = -\log(rn)/(\mu_a + \mu_s)$$

Step 3: Deflection Angle

- Deflection angle (θ) : When a photon is scattered it is deflected by this angle.

$$\cos\theta = 2* rn -1$$

Step 3: Azimuthal Angle

- Azimuthal angle (ϕ) : When deflected by the Deflection angle, it is also deflected with respect to the orthogonal plane of propagation.

$$\phi = 2 * Pi * rn$$

Step 3: Directional Cosines

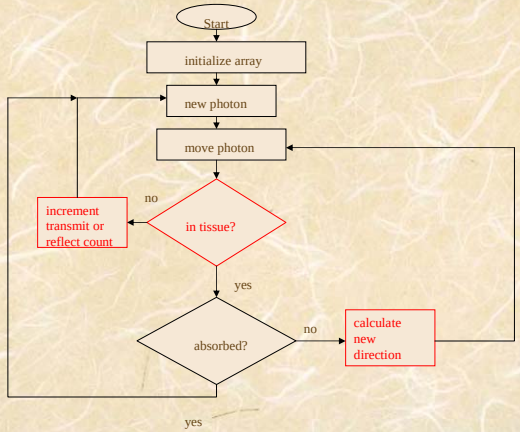
These definitions are important in the scattering concept.

- Directional cosines (u_x,u_y,u_z) : These variables keep track of which direction the photon is propagating in the tissue.
- Initial values for the trajectory are $u_z = 1$, $u_x = u_y = 0$
- The values for the trajectory after the initial step can be calculated using the formulas on the next slide

Step 3: Directional Cosines

```
If |uz|  > 0.99999
    uxprime = sin(theta)*cos(phi);
    uyprime = sin(theta)*sin(phi);
    uzprime = uz*cos(theta)/abs(uz);
else
    uxprime = sin(theta)/sqrt(1-uz*uz)*(ux*uz*cos(phi)-uy*sin(phi)) + ux*cos(theta);
    uyprime = sin(theta)/sqrt(1-uz*uz)*(uy*uz*cos(phi)-ux*sin(phi)) + uy*cos(theta);
    uzprime = -sin(theta)*cos(phi)*sqrt(1-((uz)*(uz))) + uz*cos(theta);
```

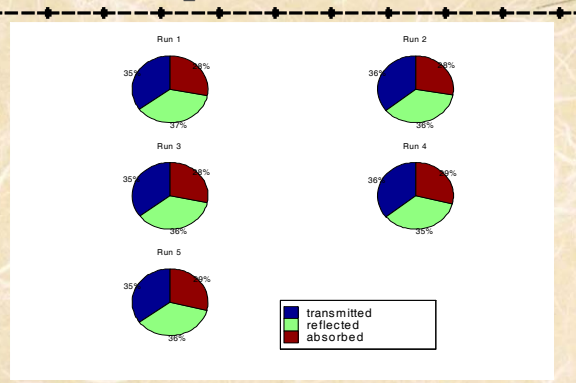
Step 3: Flow Chart



Step 3: Results

- $\mu_s = 90cm^{-1}$, $\mu_a = 10cm^{-1}$, g = 0 (isotropic);
- Tissue depth d = 0.02 cm.
- Index matched boundaries
- 5 runs of 10,000 photons
- For the above parameters, % reflected, % transmitted and % absorbed photons are displayed on the next slide

Step 3: Results



Step 4: Anisotropic Tissue and Variable Weight Photons

- Now we will consider an anisotropic medium and variable weight photons. Since some tissues tend to scatter photons in a preferred direction, the deflection angle will vary depending on the tissue.
- g (degree of anisotropy) is determined by the tissue.
- The function used to determine this is the Henyey-Greenstein function. For isotropic scattering g = 0. For all other tissues g != 0.

Step 4: Anisotropic Scattering

Definition of the Henyey-Greenstein function.

- let temp = (1 - g*g) / (1 - g + 2*g*rn)

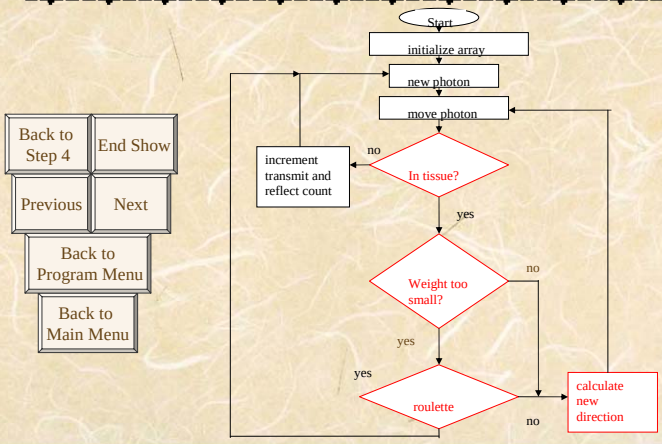
$$\theta = \text{acos}\left((1/2*g) * (1 + g*g - (\text{temp}\hat{}2)) \right)$$

Step 4: Variable Weight Photons

- Now, as a photon encounters tissue it's weight is decremented.
- Once the weight is small enough the photon will either terminate or be re-energized. A threshold is set to determine if the weight is significantly small.
- A photon is only re-energize every 1/threshold photons to keep the energy balanced. This concept is called roulette.

```
if(rn < threshold)
  weight = weight * 20;
else
  weight = 0;
```

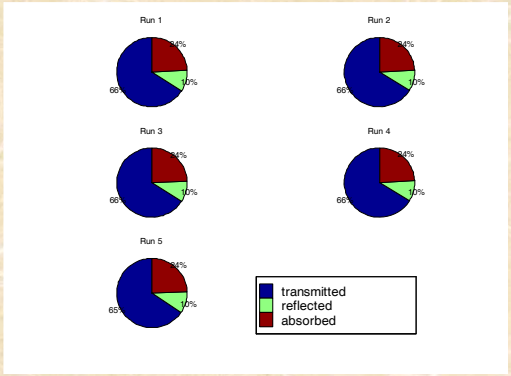
Step 4: Flow Chart



Step 4: Results

- $\mu_s = 90cm^{-1}$, $\mu_a = 10cm^{-1}$g = 0.75 (anisotropic);
- Tissue depth d = 0.02 cm.
- Index matched boundaries
- 5 runs of 10,000 photons
- For the above parameters, % reflected, % transmitted and % absorbed photons are displayed on the next slide

Step 4: Results



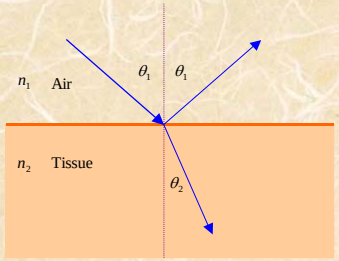
Step 5: Index Mismatch of Boundary Layers

- In this step, the index-mismatched boundary between air and tissue is taken into effect. When light enters tissue, the total reflectance R_t should include both the specular reflection R_{sp} and the remitted diffuse reflectance R_d. That is

$$R_t = R_{sp} + R_d$$

Step 5: Specular Reflection

- When a laser beam is delivered through air to tissue, a portion of the beam is reflected due to the difference in the indices of refraction, which is called specular reflection if the surface is smooth.



Step 5: Specular Reflection

- The specular reflectance r can be calculated by Fresnel's law as

$$r = \frac{1}{2}\left[\frac{\sin^2(\theta_1 - \theta_2)}{\sin^2(\theta_1 + \theta_2} + \frac{\tan^2(\theta_1 - \theta_2)}{\tan^2(\theta_1 + \theta_2}\right]$$

When the beam is normal to the surface, the above equation reduces to

$$r = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$$

- The angle of the transmitted beam is given by Snell's law as

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

Step 5: Specular Reflection

- If a photon is injected orthogonally, then the specular reflectance R_{sp} is specified as

$$R_{sp} = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$$

- And the photon weight is updated by

$$w = (1 - R_{sp})w_0$$

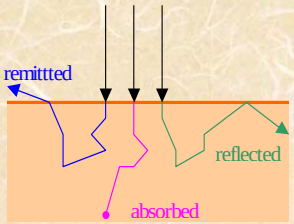
Step 5: Critical Angle

- If light within the tissue strikes the surface with an angle θ_2 greater than the critical angle θ_c, the light is totally internally reflected. The critical angle is given by

$$\theta_c = \arcsin\left(\frac{n_1}{n_2}\right) \quad \text{for} \quad n_1 < n_2$$

Step 5: Diffuse Reflection

- Some of the light scattered from the collimated beam undergoes multiple reflections and propagates.
- Backscattered light that reaches the tissue surface is either internally reflected or transmitted according to Fresnel's law.
- It is called diffuse reflection for the remitted light at the surface emerges in all directions.

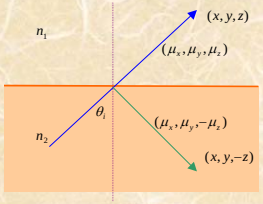


Step 5: Diffuse Reflection

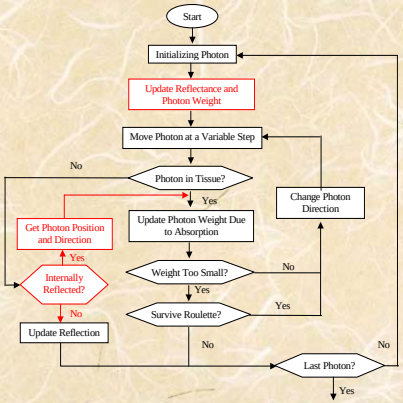
- Within the tissue, if a photon strikes the surface with an incidence angle θ_i larger than the critical angle θ_c, the photon is totally reflected.
- Otherwise, the internal reflectance $R(\theta_i)$ can be calculated by Fresnel's law.
- Generate a random number ζ. If $\zeta <= R(\theta_i)$, the photon is reflected; otherwise, the photon escapes from the tissue and its weight is added to the diffuse reflectance R_d.

Step 5: Diffuse Reflection

- When the photon is internally reflected, the z components of both position and trajectory are reversed.



Step 5: Flow Chart



Step 5: Results

- Assume a semi-infinite tissue slab with $\mu_s = 90cm^{-1}$, $\mu_a = 10cm^{-1}$, and isotropic scattering.
- Assume the indices of refraction of the air and the tissue are $n_1 = 1$, $n_2 = 1.5$, respectively.
- Use variable weight photon and variable step.
- Determine R_t using five runs of *10,000* photons.
- Compared with a theoretical value $R_t = 0.2600$ reported by Giovanelli, this model works well.

No.	1	2	3	4	5	Mean
R_t	0.2592	0.2659	0.2595	0.2630	0.2621	0.2619

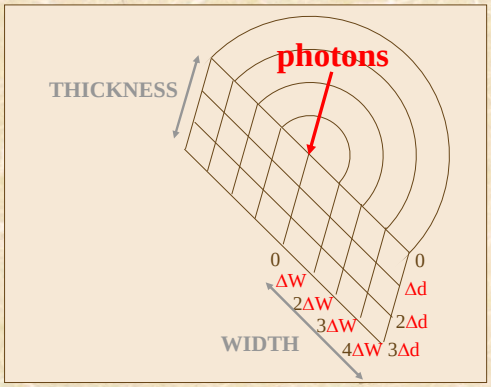
Step 6: Develop a Grid Structure

- Now we would like to keep track of the locations at which photons are absorbed within the tissue.
- To accomplish this we develop a two-dimensional array of bins corresponding to the depth of the photon and the distance it has traveled from the original axis of collimation.
- With each absorption event, the photon's weight will be added into the bin corresponding to the photon's current location.

Step 6: Grid Variables

- The necessary input variables for the structure are:
  - d dimension (also the THICKNESS of the tissue)
  - W dimension (the WIDTH of the tissue)
  - Δd resolution
  - ΔW resolution
- Our grid structure assumes a cylindrical coordinate symmetry, so radius values are calculated from: $r = \sqrt{x^2 + y^2}$

Step 6: Grid Structure Visualized

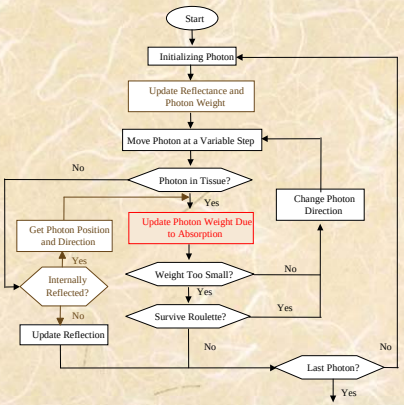


Step 6: Arrays

- Two-dimensional arrays are set up at the beginning of the program to correspond with each grid element. They are indexed with the variables I (for width) and J (for depth):
  - Absorption(I,J)
  - Source(I,J)
  - Fluence(I,J)
- A 1-D volume array is also used to calculate the I^{th} element's volume in the grid.
  - Volume(I)

Step 6: Flow Chart

All grid bookkeeping subroutines happen at the "Update Photon Weight" stage.



Step 6: Grid Bookkeeping

- Each time a photon's weight is absorbed, the grid bookkeeping subroutine must be called. The current radius value is calculated: $r = \sqrt{x^2 + y^2}$
- Array indexes are calculated by dividing the current depth (z) and radius by each corresponding resolution value:

  $I = r/\Delta W$ and $J = z/\Delta d$

Step 6: Absorbing the photon

- Part of the photon's weight is absorbed into the current grid element:

  Absorption(I,J) = Absorption(I,J) +weight* (μ_a / μ_t)

Step 6: Source Term and Fluence

- The volume of the I^{th} element is calculated:

  Volume(I) = π (2I+1) $\Delta d\ \Delta W^2$

- The source term for the current grid element is:

  Source(I,J) = Absorption(I,J) / (Volume(I)* #of Photons)

- And the fluence rate for the grid element is:

  Fluence(I,J) = Source(I,J)/ μ_a

Step 7: Finite Beam Width

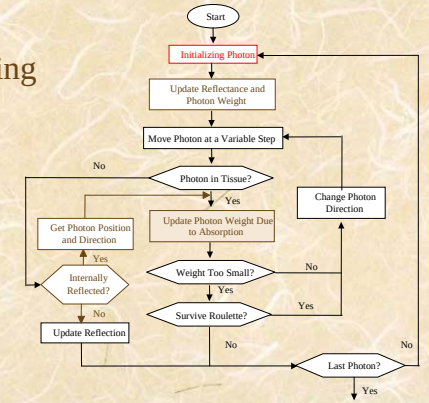
- Up to this point, all photons were launched at the origin, resulting in a ray (impulse) response. Two more typical types of beams are the uniform flat-field beam and the Gaussian beam profile.
- There are two different methods used to obtain results for different beam profiles. The first method is to distribute the incident photons according to angle and position at the time of launch. The second approach is to launch photons at the origin in order to generate an impulse response.
- The impulse response is then convolved against the appropriate beam distribution to get the desired output.

Step 7, Method 1: Distributing Photons During Initialization

- This approach is more generally applicable and can be used for asymmetric heterogeneous tissue models. The main disadvantage is that a Monte Carlo simulation must be run for each beam type or diameter.
- Assuming the tissue model is cylindrically symmetric around the z-axis, the launching of the photons may occur at y = z = 0. The beam radius (uniform beam) or $1/e^2$ radius (Gaussian beam) is defined as ω.
- Ray response: x = 0
- Uniform flat field beam: $x = \omega\sqrt{RN}$
- Gaussian beam: $x = \omega\sqrt{-\frac{\ln(1-RN)}{2}}$

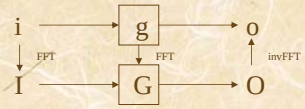
Step 7: Flow Chart

Photons are distributed during initialization.

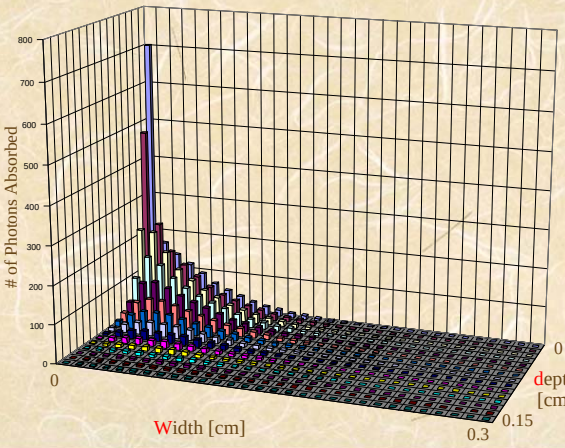


Step 7, Method 2: Convolution of Impulse Response

- The benefit of this approach is that a single Monte Carlo simulation is necessary for subsequent consideration of a variety of beam distributions. The disadvantage is that only symmetric tissue models will allow the convolution technique.
- Step 1: Obtain an impulse response from the Monte Carlo simulation. (When i=input beam distribution matrix=impulse, g=impulse response=o=output)
- Step 2: Take the fourier transform of the desired beam distribution matrix, i, and the impulse response, g.
- Step 3: Multiply the transformed matrices I and G and take the inverse FFT of the product, O, to get the desired output, o.

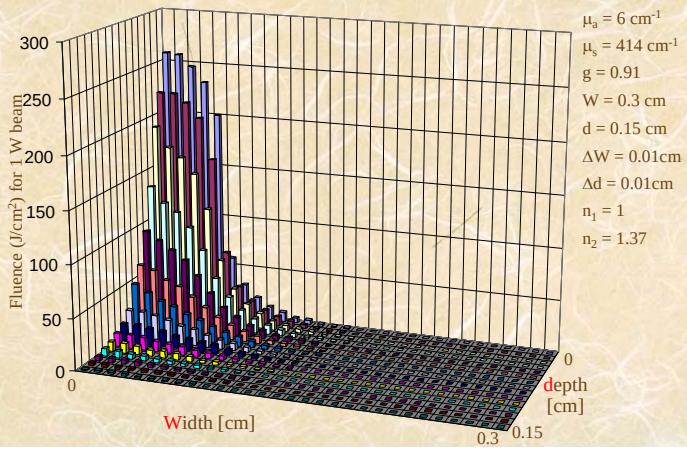


Step 7: Ray Response Results

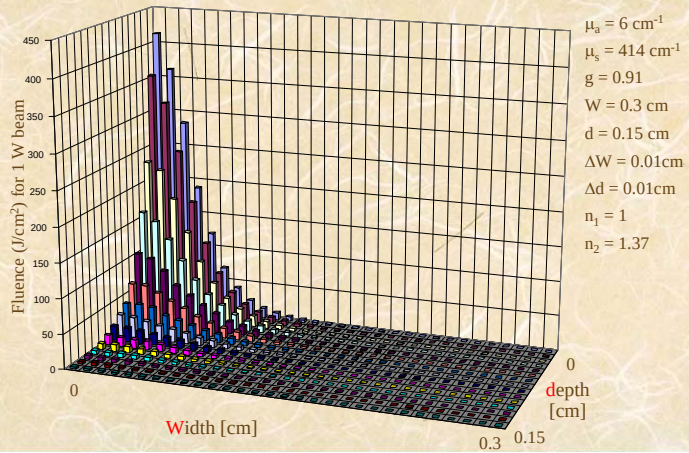


μ_a = 6 cm^{-1}
μ_s = 414 cm^{-1}
g = 0.91
W = 0.3 cm
d = 0.15 cm
ΔW = 0.01cm
Δd = 0.01cm
n_1 = 1
n_2 = 1.37

Step 7: Uniform Beam Results



Step 7: Gaussian Beam Results

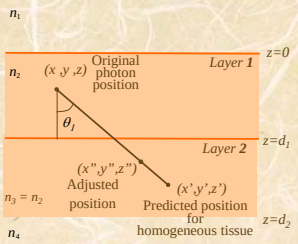


Step 8: Multiple Layer Model

- In this step we consider a multiple layer model which consist of an air interface, two layers of tissue with different optical properties (same index of refraction), and another air interface.
- The model takes into account the index-mismatched boundary between air and tissue.

Step 8: Multiple Layer Model

- When a laser beam is delivered through air to a tissue layer, part of it may be transmitted to the second tissue layer.
- In order to move a photon within the second tissue layer, first we need to determine the exact position and direction of the photon.



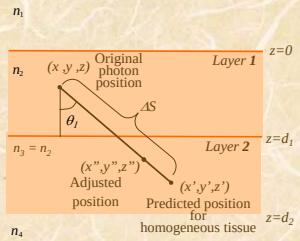
Step 8: Multiple Layer Model

- When the program determines that a photon will cross into the next tissue layer (i.e. $z' > d_1$), the total optical depth (OD) is calculated according to

  $OD = \mu_t(1) \times \Delta S$

  where ΔS is the predicted distance that the photon will travel in a homogenous layer

  $\mu_t(1)$ is the total attenuation coefficient for layer 1
- Then, we need to adjust the distance ΔS according to the total attenuation coefficient of the tissue layers.



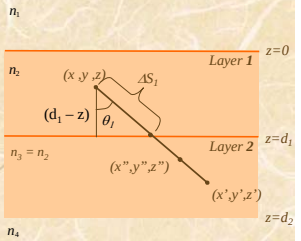
Step 8: Multiple Layer Model

- We can determine the distance that the photon travels in layer 1 (ΔS_1) because we know where the photon started (x,y,z) and the direction of travel (θ_1) to the boundary.
- Hence, $\Delta S_1 = (d_1 - z) / \cos(\theta_1)$

  where: d_1 is layer 1 thickness

  z is the initial photon position

  $\cos\theta_1$ is the photon's directional cosine.



Step 8: Multiple Layer Model

- We can define the optical depth in layer 1 as

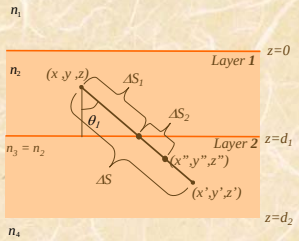
  $OD(1) = \mu_t(1) \times \Delta S_1$

  and in layer 2 as

  $OD(2) = \mu_t(2) \times \Delta S_2$
- Then, we can state that

  $\mu_t(1) \times \Delta S = \mu_t(1) \times \Delta S_1 + \mu_t(2) \times \Delta S_2$
- Finally we can solve for ΔS_2 by

  $\Delta S_2 = [\Delta S - \Delta S_1] \times [\mu_t(1) / \mu_t(2)]$



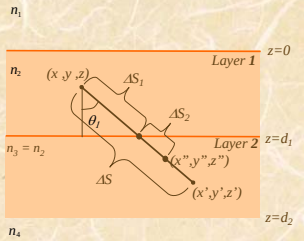
Step 8: Multiple Layer Model

- The adjusted position of the photon in layer 2 can be calculated from

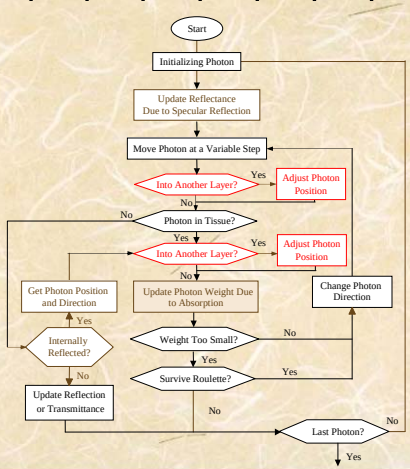
  $x'' = x + Cx * (\Delta S_1 + \Delta S_2)$

  $y'' = y + Cy * (\Delta S_1 + \Delta S_2)$

  $z'' = z + Cz * (\Delta S_1 + \Delta S_2)$



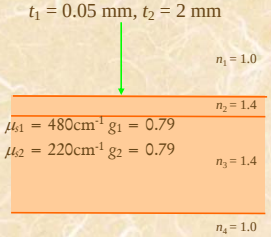
Step 8: Flow Chart



Step 8: Example

- Assume index matched between two layers of tissue
- Assume Henyey-Greenstein phase function
- Use variable weight photon and variable step
- Determine *R* and *T* using five runs of *10,000* photons
- Plot (a) Number of photons absorbed (b) Fluence rate

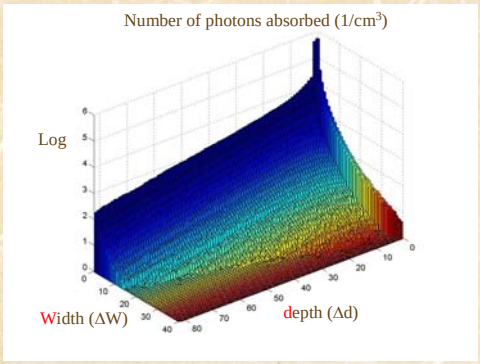
Two layers of tissue
Thickness
$t_1 = 0.05$ mm, $t_2 = 2$ mm



$\mu_{a1} = 37\text{cm}^{-1}$ $\mu_{t1} = 480\text{cm}^{-1}$ $g_1 = 0.79$
$\mu_{a2} = 2.2\text{cm}^{-1}$ $\mu_{t2} = 220\text{cm}^{-1}$ $g_2 = 0.79$

	Run1	Run2	Run3	Run4	Run5	Mean
R	0.217	0.217	0.220	0.220	0.221	0.219
T	0.011	0.013	0.013	0.012	0.013	0.012

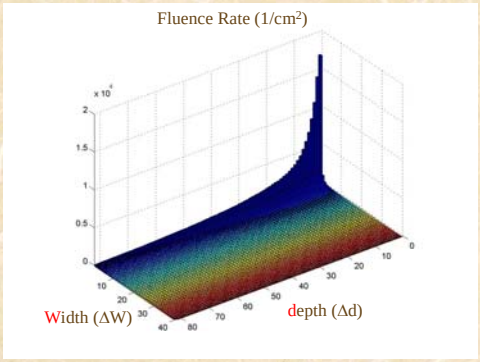
Step 8: Ray Response Results



Grid structure:
Δd = 0.025 mm
ΔW = 0.05 mm

Thickness of first layer
0.05 mm = 2 Δd

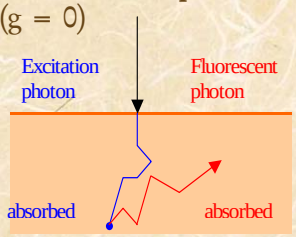
Step 8: Ray Response Results



Grid structure:
Δd = 0.025 mm
ΔW = 0.05 mm

Step 9: Fluorescence

- Absorption of excitation fluence rate $\Phi(\lambda_{ex})$ by fluorophores results in fluorescent photon with emission wavelength $\lambda_{emission} >> \lambda_{excitation}$.
- Initial spatial distribution of fluorescent photon is assumed to be isotropic (g = 0)
- Then use Henyey-Greenstein phase function



Step 9: Fluorescence

- Fluorescence proportional to number of absorption events by fluorophores
- Assume quantum yield of 1 for easier bookkeeping (one fluorescent photon for every absorbed excitation photon)
- Assume semi-infinite tissue slab

Step 9: Fluorescence

- Tissue optical properties depend on wavelength λ.
- Since excitation and fluorescent wavelengths are different ⟶ two sets of optical tissue properties

excitation wavelength

μ_a = 6.5 [cm^{-1}]
μ_s = 412 [cm^{-1}]
g = 0.89

emission wavelength

μ_a = 2.0 [cm^{-1}]
μ_s = 323 [cm^{-1}]
g = 0.89

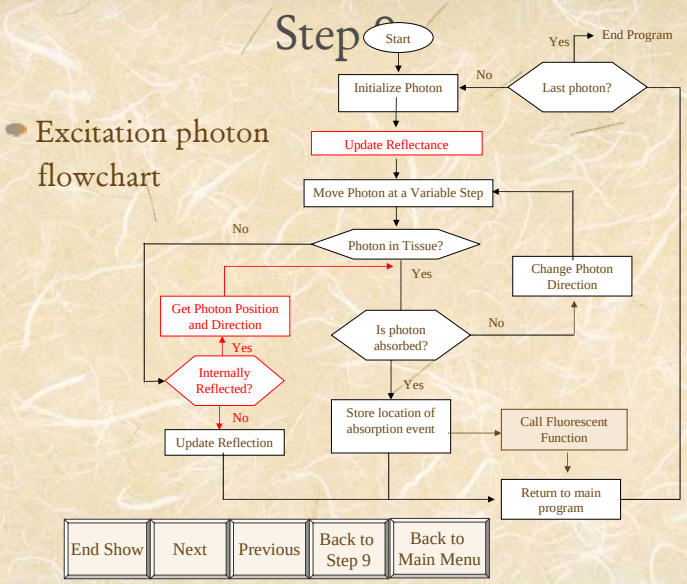
Step 9: Fluorescence

- Modeling propagation of excitation photon with fixed photon weight
- Launch photons as ray response
- Mismatched boundaries (n_{air} = 1, n_{tissue} = 1.4)
- Move and scatter photon until absorbed
- Store location of absorption event
- Initialize fluorescent photon at same location
- Modeling propagation of fluorescent photons with variable photon weight

End Show | Next | Previous | Back to Step 9 | Back to Main Menu

Step 8

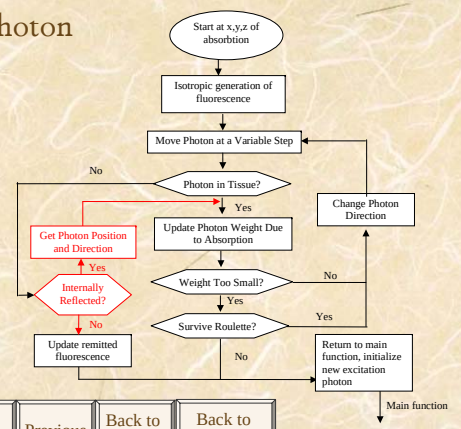
- Excitation photon flowchart



End Show | Next | Previous | Back to Step 9 | Back to Main Menu

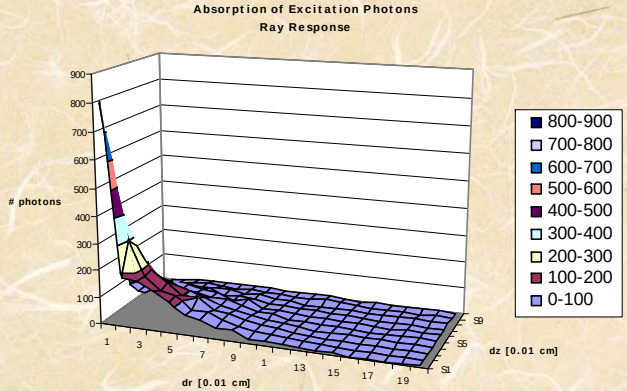
Step 9: Fluorescence

- Fluorescent photon flowchart



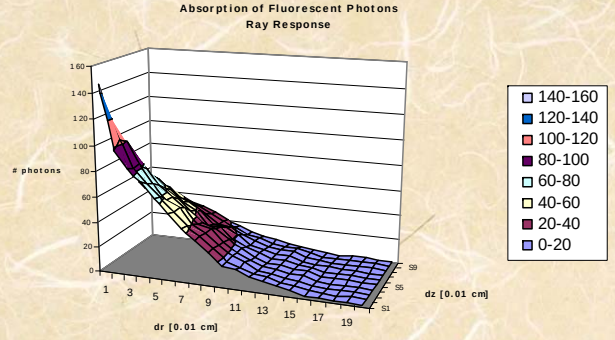
End Show | Next | Previous | Back to Step 9 | Back to Main Menu

Step 9: Fluorescence Results



End Show | Next | Previous | Back to Step 9 | Back to Main Menu

Step 9: Fluorescence Results



End Show | Next | Previous | Back to Step 9 | Back to Main Menu

Step 9: Fluorescence Results

Excitation photons	Run 1	Run 2	Run 3	Run 4	Run 5	Average
Absorbed	7689	7687	7667	7701	7666	7682
Reflected	2259	2261	2286	2253	2286	2261.2
Fluorescent photons	Run 1	Run 2	Run 3	Run 4	Run 5	Average
Absorbed	4932.66	4927.17	4947.96	4964.26	4946.96	4943.68
Reflected	2756.14	2759.70	2719.35	2737.12	2719.35	2746.19

End Show | Next | Previous | Back to Step 9 | Back to Main Menu

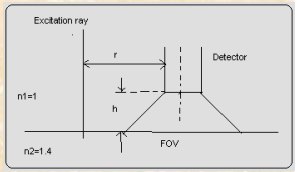
Step 10: Detection of emission photons

- The previous step involved the generation and propagation of fluorescent emission photons using variable weight Monte Carlo.
- Here we include a detector to detect the number of emission photons which enter the detector field of view.
- The detector is placed within the previously defined grid boundaries.

End Show | Next | Previous | Back to Main Menu

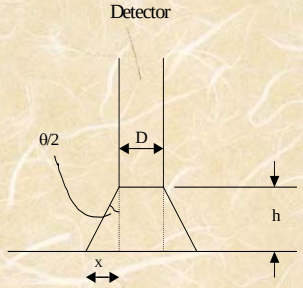
Step 10: Detector Variables

- Detector position (Lateral distance from excitation ray and the height above the tissue)
- The detector radius
- The field of view of the detector (FOV)
- If the detector is placed on the surface of the tissue, then we consider the cases of matched and mismatched boundaries.



End Show | Next | Previous | Back to Main Menu

Detection



Tan (θ/2) * h = X

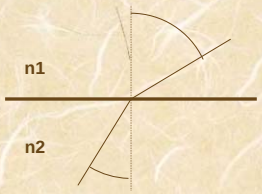
Total distance over which the photons could be detected = 2X+D

θ is the field of view

Photons here taken into consideration for detection

End Show | Next | Previous | Back to Main Menu

Directional Cosines at the Interface



Taking into account the mismatched boundaries

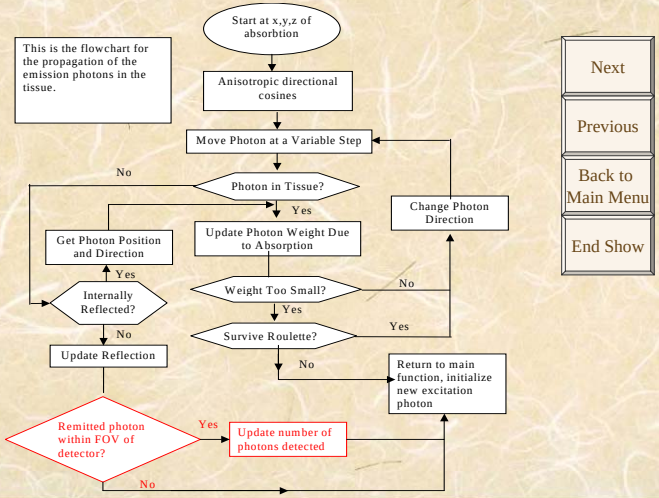
The equations to get the directional cosines are as follows

$Cx = Cxold * n2/n1$

$Cy = Cyold * n2/n1$

$Cz = \sin^{-1}(n2/n2 * \sin(\cos^{-1}(Czold)))$

Step 10: Flowchart



Step 10: Parameters for simulation

- Detector diameter set at 1,2,4,10 and 20 times Δ r of the grid.
- Consider Detector FOV of 15^0, 30^0, 60^0 and 180^0
- Use detector heights of 0, 0.1, 0.2, 0.4 and 1.0 cm
- The center of the detector is placed at 0, Δr/2, Δ r, 2 Δ r, 5 Δ r and 10 Δ r

End Show | Next | Previous | Back to Main Menu

Results 1

Height = 0cm **Position of detector=10dR** **Diameter of detector=4dR**

FOV (degrees)	Photons in FOV	Photons detected
15	27.7	26.2
30	28.1	27.2
60	28.7	27.4
180	-	28.3

End Show | Next | Previous | Back to Main Menu

Results 2

Height = 0.1 cm Position of detector=10dR Diameter of detector=4dR

FOV (degrees)	Photons in FOV	Photons detected
15	46.4	14.4
30	69.0	23.2
60	116.5	34.6
180	-	35.8

End Show | Next | Previous | Back to Main Menu

Results 3

Height = 0.2 cm Position of detector=10dR Diameter of detector=4dR

FOV (degrees)	Photons in FOV	Photons detected
15	66.2	12.6
30	109.2	21.8
60	131.4	26.4
180	-	26.2

End Show | Next | Previous | Back to Main Menu

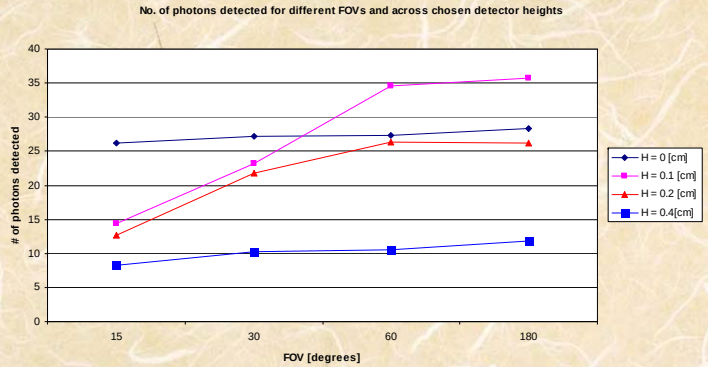
Results 4

Height = 0.4 cm Position of detector=10dR Diameter of detector=4dR

FOV (degrees)	Photons in FOV	Photons detected
15	106.8	8.3
30	129.6	10.2
60	138.6	10.5
180	-	11.8

End Show | Next | Previous | Back to Main Menu

Graphical Representation of Results



End Show | Next | Previous | Back to Main Menu

Interpretation of the results

- Number of photons detected across different heights for a particular FOV decreases
- No influence of the FOV at H = 0 cm
- Increase in detected photons with increasing FOV while H is constant

End Show | Next | Previous | Back to Main Menu

End of Monte Carlo Model

This concludes the Monte Carlo Model presentation.

End Show | Back to Main Menu | First Slide