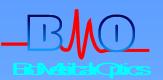


Biomedical Optics

Monte-Carlo Simulations

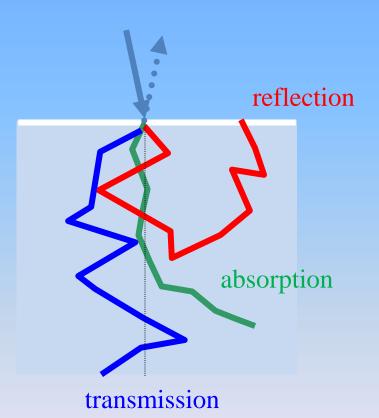
F.F.M. de Mul

(University of Twente, Enschede, the Netherlands)



Monte-Carlo simulations: Principle





Steps: Photons will be:

- 1. Emitted towards tissue
- 2. **Reflected** at surface or:
- 3. Injected into tissue;
- 4. **Propagated** over distance related to "transport mean-free-path";
- 5. Absorbed, or:
- 6. Scattered;
- 7. **Propagated** again, as in 4.
- 8. Reflected or refracted
 - at boundaries (external or internal).
- 9. Detected, when leaving the sample.

MC: Emission

Steps: Photons will be:

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.





Photon sources

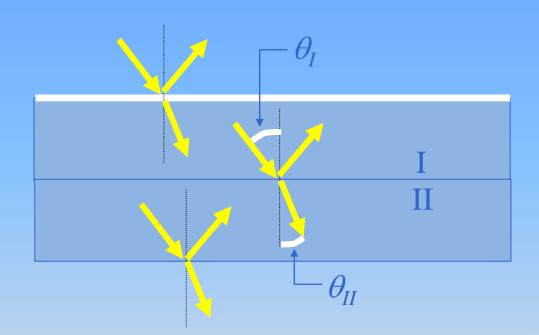
- 1. Pencil beam
- 2. Divergent beam
- 3. Tilted beam
- 4. Ring-shaped beam
- 5. Internal focus
- 6. Distributed source



MC: Reflection or Injection

Steps: Photons will be:

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.



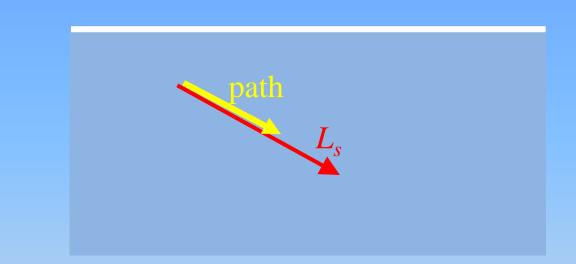
Reflection or refraction according to the Fresnel-relations: Percentage of reflection $R = f(n_I/n_{II}; \theta_{I_{\perp}}, \theta_{II})$

> In program: reflection if : *Random* * $100 \le R$ *Random* = random generator ($0 \le random < 1$)

MC: Light Propagation

Steps: Photons will be:

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.



Propagation distance determined by Lambert & Beer's Law:

I(x) = I(0). exp $(-\mu x)$; μ = attenuation coefficient

Average translation distance between scatter events: $L_s = 1 / (\mu_s + \mu_a)$; μ_s and μ_a = coefficients of the *medium*.

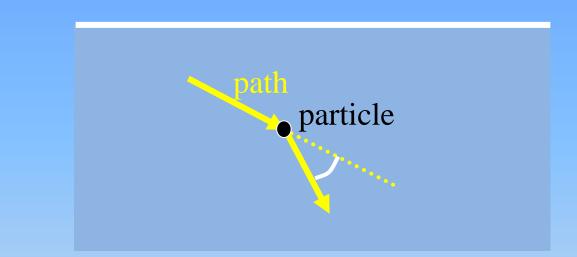
In program: $path = -L_s \cdot \ln(1-random) ; 0 \le random < 1$



MC: Absorption or Scattering

Steps: Photons will be:

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.



After propagation: arrival at particle: Absorption or Scattering

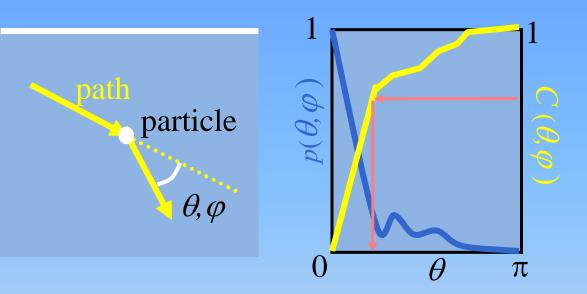
determined by absorption and scattering cross sections: σ_a and σ_s [m²] with $\mu_a = n \sigma_a$; $\mu_s = n \sigma_s$; $n = \text{nr. particles / m}^3$

In program: absorption if: $random < \sigma_a / [\sigma_s + \sigma_a]$ FdM

MC: Scattering

Steps: Photons will be:

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.



Scattering by particle: angles θ, φ determined by scattering function $p(\theta, \varphi)$ Options: isotropic, dipolar, Rayleigh-Gans, Mie,

In program: θ determined by: $random = C(\theta, \varphi)$,

 $C(\theta, \varphi)$ is cumulative scattering function

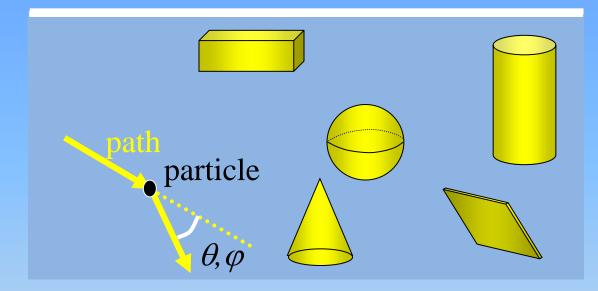
$$C(\theta, \varphi) = \int_{0}^{\theta} p(\theta', \varphi) . \sin \theta' . d\theta'$$

 φ determined by: $\varphi = random * 2 \pi$

MC: Propagation

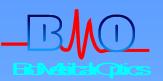
Steps: Photons will be

- 1. Emitted,
- 2. Reflected, or
- 3. Injected,
- 4. Propagated
- 5. Absorbed, or:
- 6. Scattered,
- 7. Propagated.
- 8. Reflected / refracted.
- 9. Detected.



Propagation through layers and objects Objects: options:

- rectangular blocks
- cylindrical tubes in X, Y, Z-directions or oblique
- spheres (fixed or randomly distributed)
- cones
- mirrors (one-surface only)
- torusses



1.

2.

3.

4.

5.

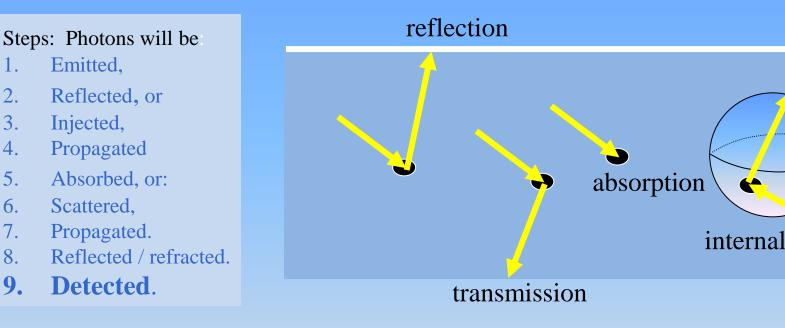
6.

7.

8.

9.

MC: Detection



Detection: options: reflection, transmission, absorption, internal

Detection window: options: XY-grid; rings; internal (sphere)



MC: Optical properties

Optical properties of tissue (at 800 nm):

	μ_a [mm ⁻¹]	μ_s [mm ⁻¹]	$g = < \cos \theta >$	n [-]	Thickn. [mm]	Scatt. func.*)	n _{rel} +) [-]
Epidermis	0.01	10	0.875	1.5	0.1	HG	1.1
Dermis	0.01	10	0.82	1.4	2	HG	1.1
Blood ^o)	1.0	70	0.99	1.4	-	Mie	1.07
Fat (subcut.)	0.001	3	0.9	1.4	0-2	Mie	≈1.1
Glass	0	0	-	1.5	-	-	-
Water	0.001	0	0	1.33	-	-	-

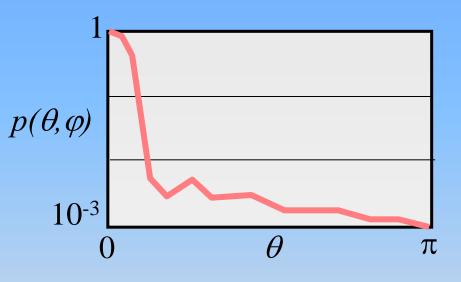
°) At hematocrit = 45 % ; Blood ≈ 1.5 vol.% in tissue *) HG = Henyey-Greenstein
+) relative refractive index of particles in medium



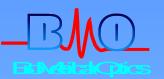
MC: Scattering functions

Scattering function: $p(\theta, \phi)$ determined by:

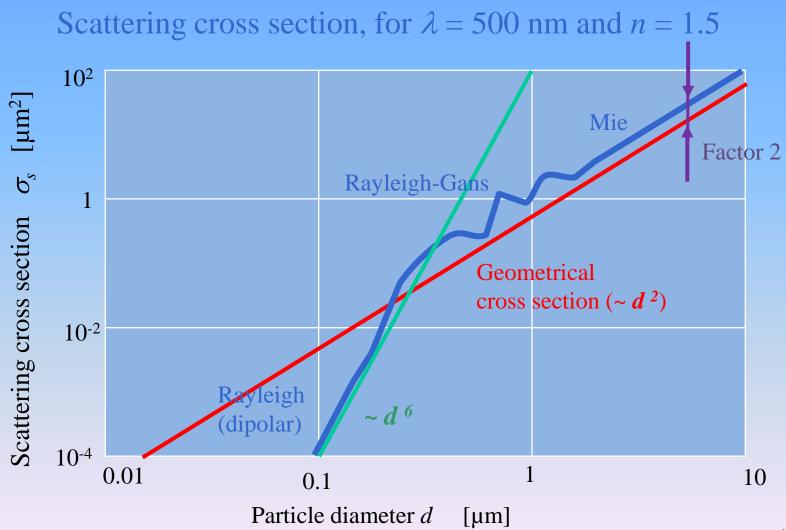
- relative refractive index n_{rel} of scattering particles in medium
- aspect ratio x = ratio of
 - particle circumference,
 - wavelength in medium



Examples	Particle sizes (λ = 800 nm)			
• isotropic	• << 0.1 μm			
• dipolar (Rayleigh)	• $0.05 - 0.2 \ \mu m$			
• Rayleigh-Gans	• 0.2 – 2 µm			
• Mie	• > 2 μm			



MC: Scattering cross section



MC: Simulations

Numerical project:

- Depart from: basic tissue structure (2-layer system)
- Use pencil beam, $\lambda = 800$ nm
- Vary one of following variables by factors 2 and $\frac{1}{2}$:
 - 1. Thickness of epidermis
 - 2. Thickness of dermis
 - 3. Scattering coefficient of dermis
 - 4. Absorption coefficient of epidermis
 - 5. Scattering coefficient of epidermis, or
 - 6. Scattering function
- Calculate: I(r) for source-detector distance r = 0...3 mm, normalize to 1 at r = 1 mm
- Plot: $\ln I(r)$ vs. *r* and calculate μ_{eff}
- Compare μ_{eff} with monolayer situation (dermis only)

MC - program

How to handle the Monte-Carlo-program:

- Depart from: Creation of Scattering Functions (*.MIE-files)
- Create Input data-files (*.INP-files).
- If more (related) simulations wanted: create List of INP-files (*.LST-file)
- Start Simulations
- After completion of simulations: results in *.FOT-files Plot: ln *I* (*r*) vs. *r* for *r* = 0..3 mm (plot option available in program).
- Calculate μ_{eff} and compare with monolayer situation (dermis only)



Monte-Carlo simulations

The end