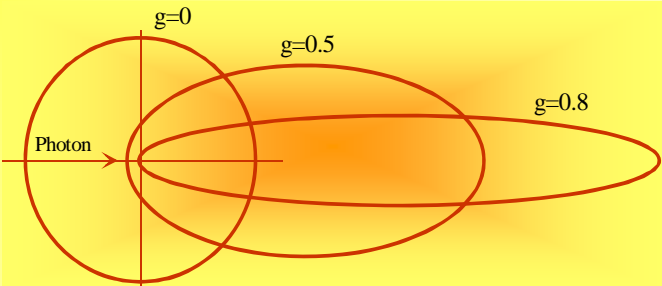


Monte Carlo simulations to predict light transport in turbid media



Photon

$g=0$

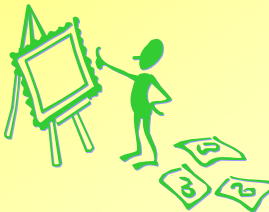
$g=0.5$

$g=0.8$

Medical Optics

Stefan Andersson-Engels

Monte Carlo (MC) Simulations



The outline of this presentation is

- Introduction
- Discuss how to randomise the parameters
- Briefly describe the calculations of step size and trajectory directions
- Describe the result files
- Outline how one can handle distributed sources

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Monte Carlo Simulations

Monte Carlo simulations are frequently used to model propagation of light in tissue.

This model is based on random walk, where a photon or a photon package is traced through the tissue until it exits or is terminated due to absorption.

By repeating this process for a large number of photon packages, it is possible to obtain statistics for these physical quantities.

Many physical parameters of the photon package can be logged, e.g. the distribution of absorption, exiting position, time-of-flight etc.

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Monte Carlo Simulations

Main advantage

- no limitation concerning boundary conditions or spatial localisation of inhomogeneities in the tissue

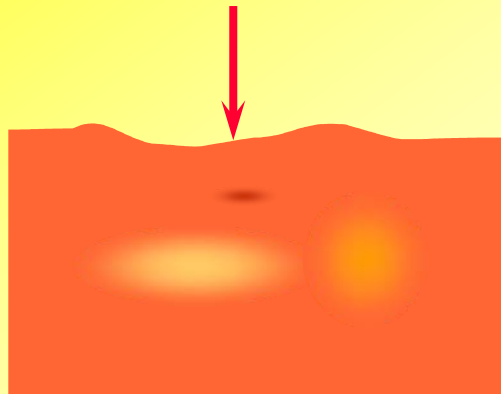
Main disadvantage

- problem of getting good statistics, particularly if the point of interest is located far away from the point of entry of the light and the scattering and absorption coefficients are high.

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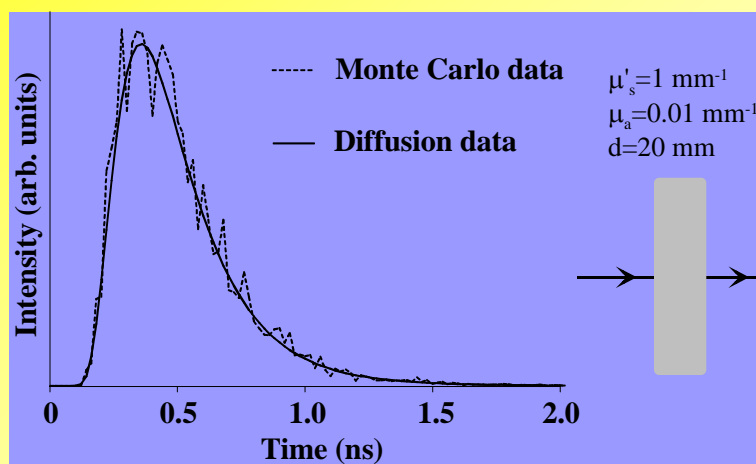
MC can handle **any** geometry

Incident light



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An example of an MC simulation



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Available Monte Carlo codes

A public domain computer code (MCML), written by Wang and Jacques treats the steady state case for a multi-layered medium.

MCML can provide steady-state results for the distribution of escaped as well as absorbed light in a multi-layer geometry.

Many developed versions based on this code are used by various groups around the world.

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Monte Carlo Simulations

- Monte Carlo simulations of photon propagation offer a **flexible approach** to predict photon transport in turbid media.
- It is based on the transport equation.
- No further assumptions are made.
- Macroscopic parameters characterising the medium is used.

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Monte Carlo Simulations

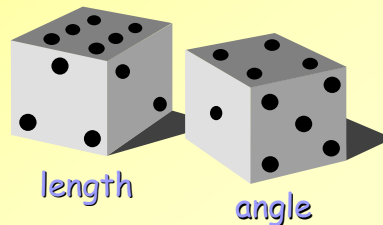
- Monte Carlo simulations can be used for simulating all kinds of particle transport. It has mainly been developed for neutron transport in combination with nuclear reactions.
- For light transport in turbid media we consider photons as neutral particles and neglect all wave phenomena.

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Monte Carlo Simulations

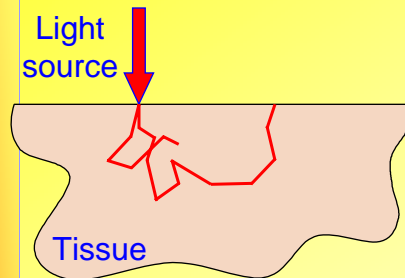
- It is as the name implies a method that relies on random sampling of propagation variables from well defined probability distributions
- The path length before a scattering or an absorption event occur
- The scattering angle

“throwing the dice”



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Light transport in tissue



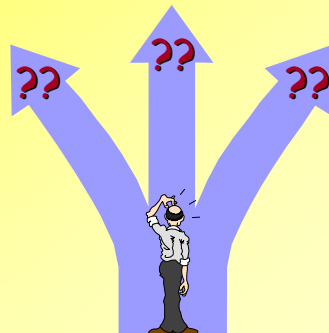
- Path length
- Scattering direction
- Absorption

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Monte Carlo (MC) Simulations

The outline of this presentation will be

- Introduction
- **Discuss how to randomise the parameters**



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How to sample random variables 1

Consider a random variable x needed for a Monte Carlo simulation. Then there is a probability density function $p(x)$ of x , which defines x over the interval $a \leq x \leq b$ such that:

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

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How to sample random variables 2

The probability that x will fall in the interval $[a, x_1]$ is given by the distribution function $F_x(x_1)$, defined as:

$$F_x(x_1) = \int_a^{x_1} p(x) dx$$

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How to sample random variables 3

By using a random number generator, one can obtain a random number ζ in the range $[0, 1]$.

The probability density function for this random number is 1 in the range $[0, 1]$.

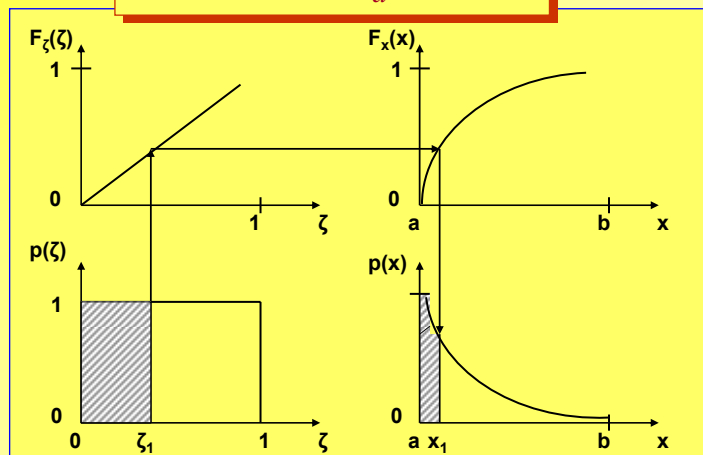
The corresponding probability distribution is

$$F_{\zeta}(\zeta_1) = \int_0^{\zeta_1} p(\zeta) d\zeta = \zeta_1 \quad 0 \leq \zeta_1 \leq 1$$

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How to sample random variables 4

This method gives the value $\zeta = F_x(x) = \int_a^x p(x) dx$ for a randomly picked value x that is:



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Monte Carlo (MC) Simulations

The outline of this presentation will be

- Introduction
- Discuss how to randomise the parameters
- **Briefly describe the calculations of stepsize and trajectory directions**

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Selecting the step size, s

The step size is in the interval $[0, \infty]$.

The probability for a photon to interact in the interval $[s_1, s_1+ds_1]$ is $\mu_t ds_1$. This means that the intensity I of the light that has not interacted with the medium decreases in the interval ds_1 by

$$\frac{dI(s_1)}{ds_1} = -\mu_t I(s_1)$$

$$p(s_1) = \frac{I_s}{I_0} = \mu_t \exp(-\mu_t s_1)$$



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Selecting the stepsize, s

The cumulative distribution function for free path s is then:

$$P\{s < s_1\} = 1 - \exp(-\mu_t s_1)$$

yielding a probability density function

$$p(s_1) = \frac{dP\{s < s_1\}}{ds_1} = \mu_t \exp(-\mu_t s_1)$$

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Selecting the step size, s

As we already know:

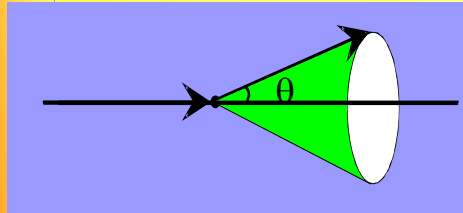
$$\zeta = \int_0^s p(s) ds = \int_0^s \mu_t \exp(-\mu_t s) ds = 1 - \exp(-\mu_t s)$$

By rearranging this we get:

$$s = \frac{-\ln(1 - \zeta)}{\mu_t} = \frac{-\ln(\zeta)}{\mu_t}$$

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Phase function symmetry



- The phase function has an axial symmetry and depends only on the angle θ .
- Often the phase function is expressed as a function of the cosine of the scattering angle - $p(\cos \theta)$

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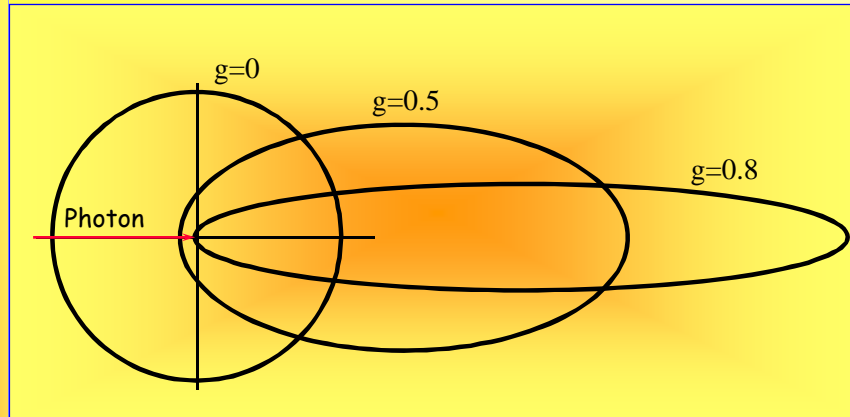
Selecting the deflection angle

- θ is in the interval $[0, \pi]$
- For convenience we will consider $\mu = \cos(\theta)$
- μ will be distributed in the interval $[-1, 1]$
- For Mie scattering the Henyey-Greenstein is a good approximation for the probability density function:

$$p(\mu) = \frac{1 - g^2}{2(1 + g^2 - 2g\mu)^{3/2}}$$

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The Henyey-Greenstein function



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Selecting the deflection angle

By using equations derived earlier we get:

$$\zeta = \int_{-1}^{\mu} p(\mu) d\mu = \int_{-1}^{\mu} \frac{1-g^2}{2(1+g^2-2g\mu)^{3/2}} d\mu$$

After solving this for μ we have:

$$\mu = \frac{1}{2g} \left[1+g^2 - \left(\frac{1-g^2}{1-g+2g\zeta} \right)^2 \right] \quad \text{for } g \neq 0$$

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Selecting the deflection angle

As g approaches zero it is not possible to express as $\mu=\mu(z)$ -- the equation becomes undefined. Instead one can use that the probability density function becomes isotropic $p(\mu)=1/2$. This yields:

$$\zeta = \int_{-1}^{\mu} \frac{1}{2} d\mu = \frac{1}{2}(\mu+1) \quad \text{or} \quad \mu = 2\zeta - 1 \quad \text{for } g=0$$

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Selecting the azimuthal angle

The azimuthal angle is uniformly distributed within the interval $[0, 2\pi]$. Thus we have

$$\zeta = \int_0^{\psi} \frac{1}{2\pi} d\psi = \frac{\psi}{2\pi}$$

This gives ψ in the form:

$$\psi = 2\pi\zeta$$

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Launching a photon package

- We start with launching a photon package assigned with a weight W , equal to unity.
- The photon package is injected orthogonally into the tissue at the origin, corresponding to a collimated ray of incident photons.
- Some specular reflection will occur if there is a mismatched boundary - $W=1-R$

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Photon absorption

During each step some attenuation of the photon package weight occur due to absorption.

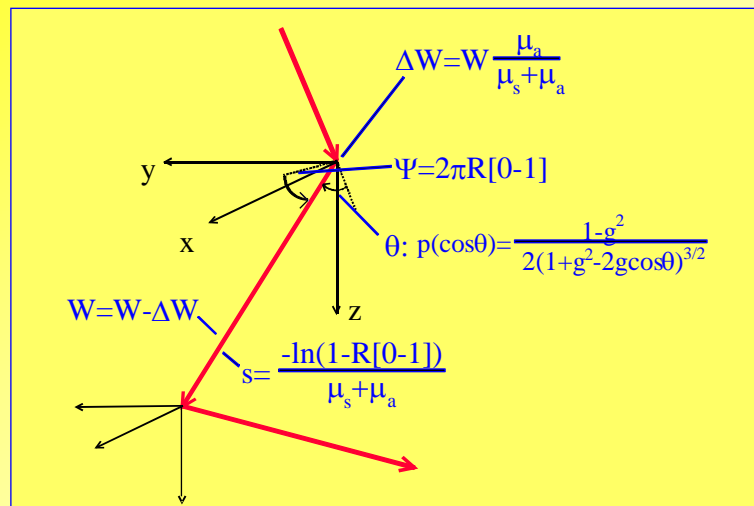
The deposited energy is $\Delta Q = W \frac{\mu_a}{\mu_t}$

and the new photon weight is $\Delta W = W \frac{\mu_s}{\mu_t}$

(note that $\Delta Q + \Delta W = W$)

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How each step is randomised



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Internal reflectance or escape

For each step one has to check if the photon package crosses a boundary (internal/external).

If this is the case one has to check for internal reflectance and/or escape. This is calculated using the Snell and Fresnel laws.

The escaped fraction adds to the result file and reduces the weight of the photon package left.

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Moving the photon package

- Specify the step size s as described
- The current trajectory direction is \mathbf{r} yielding

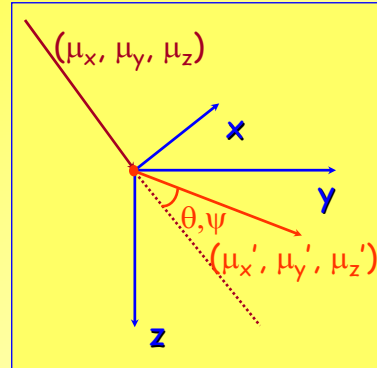
$$\begin{aligned} \mu_x &= \mathbf{r} \cdot \mathbf{x} \\ \mu_y &= \mathbf{r} \cdot \mathbf{y} \\ \mu_z &= \mathbf{r} \cdot \mathbf{z} \end{aligned} \quad \text{resulting in} \quad \text{new positions}$$

$$\begin{aligned} x' &= x + \mu_x s \\ y' &= y + \mu_y s \\ z' &= z + \mu_z s \end{aligned}$$

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Scattering direction

Rotation of the coordinate system yields



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

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

$$\mu'_z = -\sin \theta \cos \psi \sqrt{1 - \mu_z^2} + \mu_z \cos \theta$$

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Photon package termination

After a certain number of scattering events the remaining photon package weight will be low.

It is certainly a waste of time to follow this package once it has a weight lower than a pre-set threshold W_{th} .

The algorithm used to have an efficient MC code, is to use a technique called roulette.

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Photon package termination

The termination of a photon package must ensure conservation of energy.

Assume a photon package with a weight $W < W_{th}$:

- The roulette technique gives a package a chance of m of surviving with a weight mW .
- Otherwise the weight is reduced to zero and the package is terminated.

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Monte Carlo (MC) Simulations

The outline of this presentation will be

- Introduction
- Discuss how to randomise the parameters
- Briefly describe the calculations of step size and trajectory directions
- **Describe the result files**

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Recording of results

Depending on what one want to achieve the simulation the results recorded might differ.

One has to define the type of matrix in which the results should be recorded. The resolution of the grids determine the size of the matrix.

Results can be recorded as **absorbed**, **reflected** or **transmitted** fraction.

These functions can be recorded as a function of **position**, **trajectory direction** and **time**.

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Monte Carlo (MC) Simulations

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- **Outline how one can handle distributed sources**

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Distributed source handling

- ➔ Launch photon packages as over the area illuminated.
 - ➔ Flat-field beam
 - ➔ Gaussian beam
- ➔ Use pencil beam simulation and use this as a Green function and convolute with the real illumination profile to obtain the results sought.

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Checking your results

How do you know that your computer code solves your problem?

The code will always produce some numbers, but are they correct?

→ Check the code against results already published!

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Why Monte Carlo?

- ↗ **Provides accurate prediction of light fluence in tissue**
- ↗ **Can be used for complex geometries and without restrictions in optical properties**

Drawbacks with Monte Carlo

- ↗ **Does not provide any analytical expression with functional dependence of parameters of interest**
- ↗ **Large computer capacity required**
- ↗ **Fluorescence Monte Carlo requires especially long simulation times, as this often involves many wavelengths**

Important applications

- ↗ **Dosimetry in connection to PDT of skin lesions**
- ↗ **Fluorescence diagnostics of early malignant tumours**
- ↗ **etc**

Intrinsic fluorescence

It is often of interest to be able to measure the intrinsic fluorescence properties independent on the light propagation in the medium

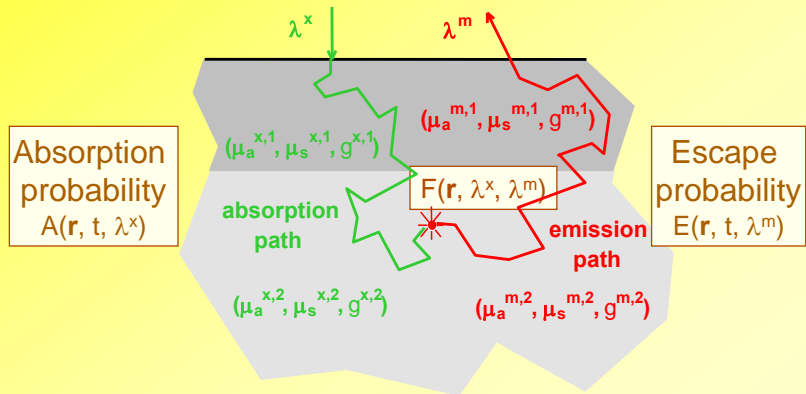
- can compare with properties in solutions
- is independent of the measurement geometry
- decrease the influence of various tissue parameters

New development of MC

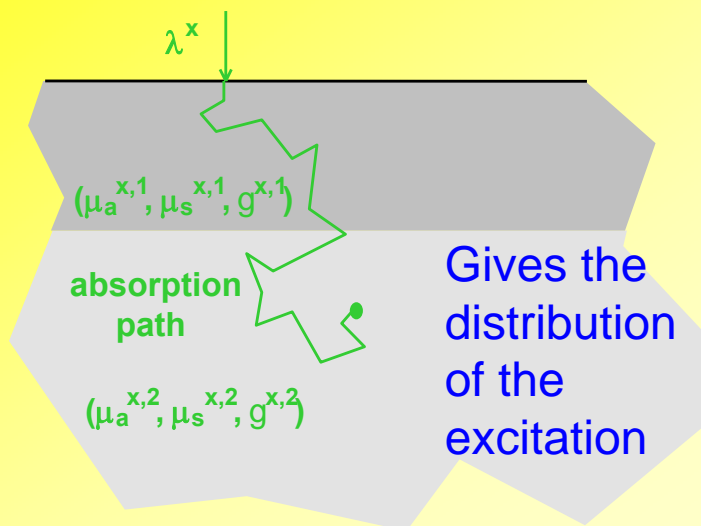
To reduce the computation time, different, modified Monte Carlo models can be used.

A condensed Monte Carlo model can simulate the light distribution for one set of optical properties and scale the results to other optical properties.

One novel MC model is developed to extract the intrinsic fluorescence properties from measurements of thin layered tissue structures



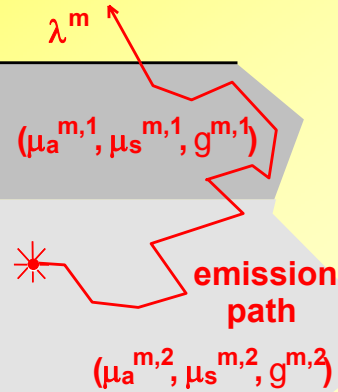
Absorption probability $A(r, t, \lambda^x)$



Escape probability $E(r, t, \lambda^m)$

Yields the probability that light emitted at position r will be detected at the tissue surface

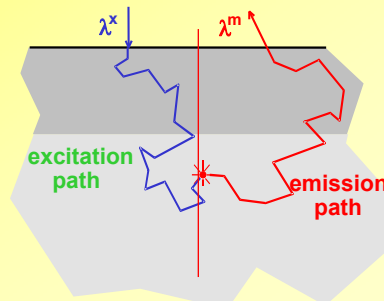
$F(r, \lambda^x, \lambda^m)$ is the intrinsic fluorescence quantum yield at position r



Standard Fluorescence Monte Carlo - Simulate each photon until it is absorbed and then follow the fluorescence photon

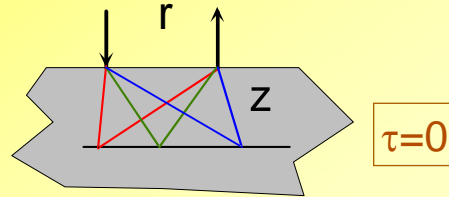
"Forward" Monte Carlo - Simulate $A(r, t, \lambda^x)$ and $E(r, t, \lambda^m)$ independently and convolve these probabilities in time and space for a fixed depth z

"Reverse" Monte Carlo - An approximate expression for the escape function can be calculated by studying the reverse path, from the surface down in the medium



“Forward” Monte Carlo

With a convolution in space and time for a fixed depth z , the escape function needs only to be simulated along the z -axis.

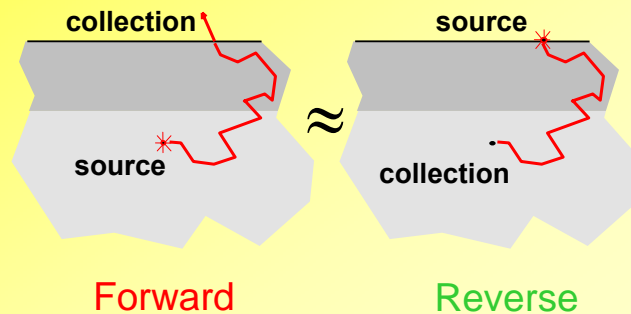


$$I_F(r, t, z) dz =$$

$$= dz \int_0^\infty r' dr' \int_0^{2\pi} d\varphi' \int_0^\infty A(r', t', z) E(r'-r, t'-t, z) dt'$$

“Reverse” Monte Carlo

The equivalence between the forward and the reverse approach for the simulation of the photon path is depicted. The main discrepancies are expected at the interface between two layers with different refractive indices

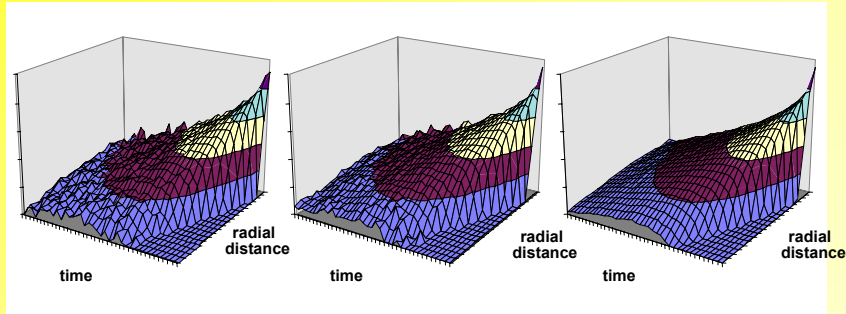


Results

Standard

Forward

Reverse



Radial distribution of the surface fluorescence

Values used

$$\mu_a^x = 2.0 \text{ cm}^{-1}$$

$$\mu_a^m = 0.5 \text{ cm}^{-1}$$

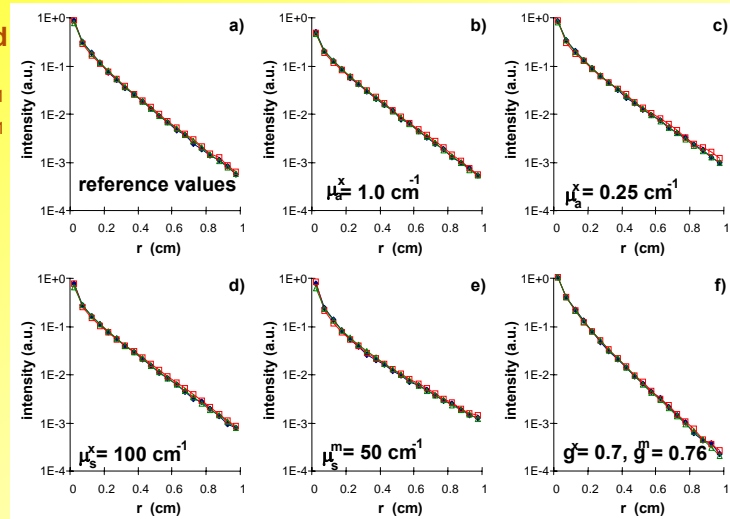
$$\mu_s^x = 100 \text{ cm}^{-1}$$

$$\mu_s^m = 50 \text{ cm}^{-1}$$

$$g^x = 0.8$$

$$g^m = 0.84$$

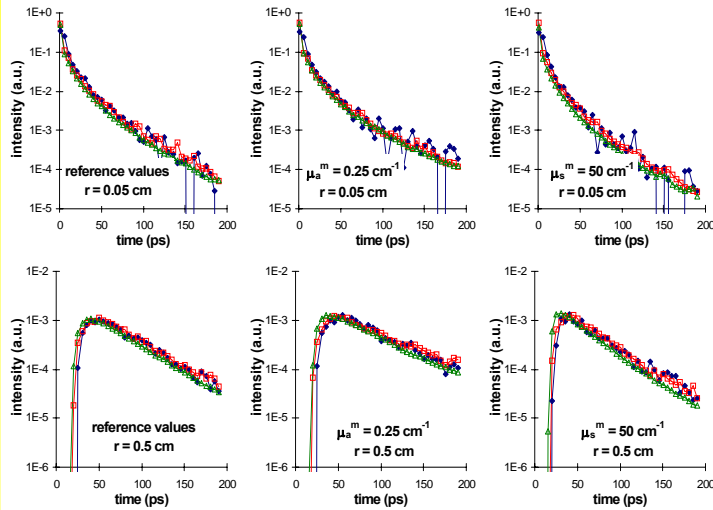
$$\tau = 1 \text{ ps}$$



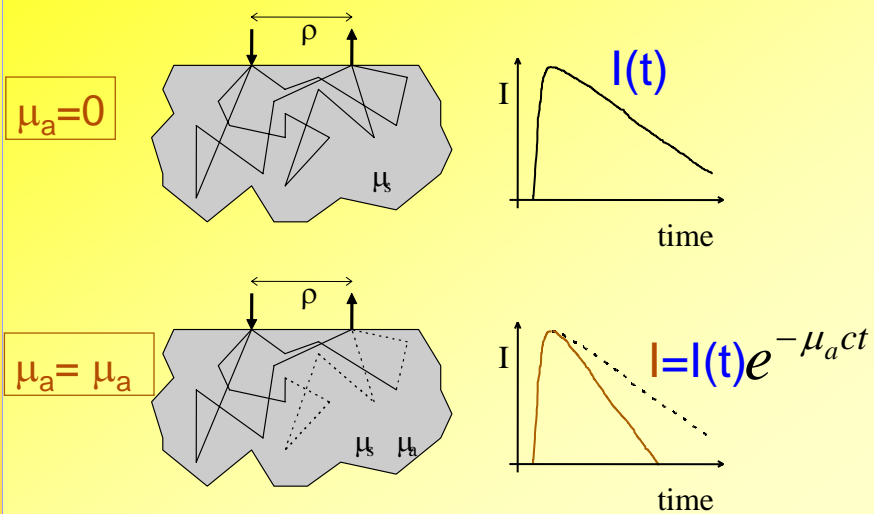
Time-resolved surface fluorescence

Values used

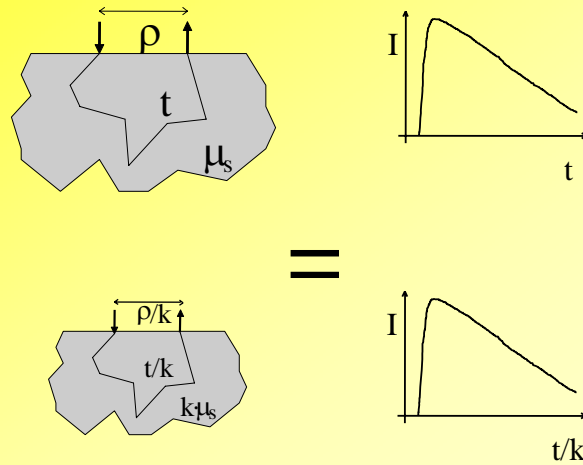
$\mu_a^x = 2.0 \text{ cm}^{-1}$
 $\mu_a^m = 0.5 \text{ cm}^{-1}$
 $\mu_s^x = 100 \text{ cm}^{-1}$
 $\mu_s^m = 50 \text{ cm}^{-1}$
 $g^x = 0.8$
 $g^m = 0.84$
 $\tau = 1 \text{ ps}$



White Monte Carlo



Scaling of scattering properties



Example of required simulation times

- Simulation times for 100 kphotons
 - SMC 470 sec
 - FMC 650 sec Convolution 40 sec
 - RMC 580 sec Convolution 40 sec
 - WMC 810 sec Convolution 40 sec
- Number of photons required for the same photon noise
 - SMC 512kp, FMC 64 kp, RMC 4 kp

Conclusions

- RMC an order of magnitude faster than FMC, which is again approximately 10 times faster than SMC
- Fluorescence distributions very similar for the 3 models
- Time resolved fluorescence distributions similar for not too short times
- Absolute fluorescence intensities still not accurate for either of the new models