# PHOTON TRASPORT WITH THE MONTE CARLO METHOD

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## 1. Introduction

### Foundations of the Monte Carlo method

Random number generation using congruntial generators

In the computer, the random numbers $\xi$ are generated artificially using mathematical formulas called "congruentials"

$$x_{n+1} = \lambda x_n + b \quad (mod\, P)$$

where P is generally $2^\beta$ or $10^\beta$, with $\beta$ the bit length of the "machine word".
Such a generators produce random integers belonging to the interval (0,T), where T is the largest integer allowed on the machine (for example, $T=2^{\beta-1}-1$ on a binary computer).

Real random numbers in the interval (0,1] can be obtained by computing : $\xi_n = \frac{x_n}{T}$

As an example, a good generator for a 32 bit computer is given by:

$\lambda$=1812433253
$P=2^{32}$
b=odd integers
$T=2^{31}-1=2147483647$

Some properties that pseudo random numbers must verify

- indistinguishable from true random numbers
- uniformly distributed in the interval (0,1]
- uncorrelated
- non repeatable

The Monte carlo method as a technique for computing integerals

Numerically, a defined integral is always computed by using the quadrature formula

$$\int_a^b f(x)dx \cong \sum_{i=1}^{N} \omega_i f(x_i)$$

By assigning the same weight $\omega_i = \frac{b-a}{N}$ to each node $x_i = (b-a)\xi_i + a$

it can be obtained $\int_a^b f(x)dx \cong (b-a)\frac{\sum_{i=1}^{N} f(x_i)}{N} = (b-a) < f >$, where <f> represents the mean value of the function f in the integration interval.

For such an expression the statistical error is given by the standard deviation

$$\sigma_I = (b-a)\sqrt{\frac{< f^2 > - < f >^2}{N}}$$

Finally, the integral can be written as

$$\int_a^b f(x)dx \cong (b-a)\left(< f > \pm \sqrt{\frac{< f^2 > - < f >^2}{N}}\right)$$

Comparison with other methods of numerical integration

The Monte Carlo method is very inefficient as a numerical technique since the error is given by $\sigma_I \propto \frac{1}{\sqrt{N}}$.

This means that an improvement of one significant figure in the result ($\frac{\sigma_I}{10}$), is necessary to use a number of nodes (random numbers) which is 100 times greater.

Compared to deterministic methods, the **truncation error** of the Monte Carlo method is decisively **worst** than that of other methods used for numeric integration.

| Method | Error |
|---|---|
| Monte Carlo | $N^{-1/2}$ |
| Trapezoidal rule | $N^{-2}$ |
| Simpson | $N^{-4}$ |

Validity of the method for computing multidimensional integrals

However, the Monte Carlo method (which maintains the same form for multidimensional integrals) shows to be more convenient than other deterministic methods of integration, from dimension 6-7 or higher.

## 2. The Monte Carlo method as a simulation technique for radiation transport

Advantages: Allows the treatment of transport problems
In special geometries
In real situations (for instance, by considering in detail an apparatus or an experimental device that can be composed by parts of different shapes and materials)
Coupled (combined transport of different species of particles)
With many collisions (what makes it indicated for treating multiple scattering problems, see figure 1)

Disadvantages: it remains always an statistical method, with an associated error.

### 2. 1. The Monte Carlo method as an statistical technique

The function density of probability for a certain event: definition

If p(x)dx is the probability of finding the variable x in the interval (x, x+dx), with $a \leq x < b$, it is obviously verified that:

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

p(x) is called **probability density**

Probability of an event

The probability P varies from 0 to 1, depending on the value of x, and is given by

$$\xi = P(x) = \int_a^x p(x)dx$$

from which it is possible to determine $x=x(\xi)$.

Example

Let us consider particles which are distributed evenly in the interval [a,b)

Then, we have

$$p(x)dx = \frac{dx}{b-a}$$

which verifies the property

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

By appling the probability formula it is possible to obtain

$$\xi = P(x) = \int_a^x p(x)dx = \int_a^x \frac{dx}{b-a} = \frac{x-a}{b-a}$$

from which we can see that the expression

$$x = (b-a)\xi + a$$

determines x as a function of the random number $\xi$.

Note that this result was applied for computing the integral in the preceding section.

## 2.2. Study of a simple case: attenuation of a photon beam in a medium of infinite thickness

Transport equation with only the soruce and attenuation terms

The transport equation for a photon source, monochromatic and monodirectional, in 1-D is given by

$$\omega_z \frac{\partial f}{\partial z} = -\mu f + I_0 \delta(\vec{\omega} - \vec{\omega}_0)\delta(\lambda - \lambda_0)\delta(z)$$

This has as a solution

$$f = \frac{I_0}{|\omega_z|}\delta(\vec{\omega} - \vec{\omega}_0)\delta(\lambda - \lambda_0)\, exp\left[-\frac{\mu|z|}{|\omega_z|}\right]\frac{(1 + sgn(z)\,sgn(\omega_z))}{2}$$

which for $z>0$, $\omega_{0z} > 0$ takes the well known expression

$$f = \frac{I_0}{\omega_z}\delta(\vec{\omega} - \vec{\omega}_0)\delta(\lambda - \lambda_0)\, exp\left[-\frac{\mu z}{\omega_z}\right]$$

which is equivalent to

$$I = I_0\, exp\left[-\frac{\mu z}{\omega_{0z}}\right]$$

At which depth the first interaction will occurs?

To answer this question we write the probability to have the first collision between z and z+dz

$$p(z)dz = exp\left[-\frac{\mu z}{\omega_{0z}}\right]\frac{\mu}{\omega_{0z}}dz$$

which verifies the property

$$\int_0^{\infty} p(z)dz = 1.$$

By applying the probability formula, we obtain that the probability for some collision taking place at a depth $z \le t$ is

$$\xi = P(t) = \int_0^t p(z)dz = \frac{\mu}{\omega_{0z}}\int_0^t exp\left[-\frac{\mu z}{\omega_{0z}}\right]dz = 1 - exp\left[-\frac{\mu t}{\omega_{0z}}\right]$$

from which we obtain the depth t

$$t = -\frac{\omega_{0z}}{\mu} ln(1 - \xi)$$

which is better known with the aspect

$$t = -\frac{\omega_{0z}}{\mu} ln(\xi)$$

## 2.3. A small complication on the preceding case: attenuation of the beam across a finite thickness.

Transport equation with only the source and attenuation terms, identical to the preceding case.
The difference is that in this case the material has a finite thickness d, and therefore the expression

$$I = I_0 \, exp\left[-\frac{\mu z}{\omega_{0z}}\right]$$

has validity only for $0 \le z \le d$. Let us imagine to have vacuum outside of this material, in such a way that the beam cannot undergone further attenuation after it has crossed the thickness d.

Formula for the forced first collision.
As in the preceding case, the probability to have the fist collision between z and z+dz is

$$p(z)dz = exp\left[-\frac{\mu z}{\omega_{0z}}\right]\frac{\mu}{\omega_{0z}}dz .$$

In this case the normalization property is nor more verified , but else

$$\int_0^{\infty} p(z)dz = 1 - exp\left[-\frac{\mu d}{\omega_{0z}}\right] < 1$$

By applying the formula above, the probability of a collision taking place at a thickness $z \le t \le d$ is

$$\xi = P(t) = \int_0^t p(z)dz = \frac{\mu}{\omega_{0z}}\int_0^t exp\left[-\frac{\mu z}{\omega_{0z}}\right]dz = 1 - exp\left[-\frac{\mu t}{\omega_{0z}}\right]$$

from which it is possible to obtain t

$$t = -\frac{\omega_{0z}}{\mu} ln(\xi)$$

This result agrees the hypothesis of the physical model but it leaves us a doubt:
in all the cases in which the photon is not attenuated in the thickness (transmission case), the computation of the depth is not necessary because it is well known that the transmitted fraction is

$$exp\left[-\frac{\mu d}{\omega_{0z}}\right]$$

To avoid to loose time with the photons that cannot interact, it is introduced the concept of weight W, with which it is considered only the fraction of photons that can interact in the thickness d:

$$W = 1 - exp\left[-\frac{\mu d}{\omega_{0z}}\right]$$

Clearly, for all the photons belonging to the fraction W, it must be verified the following property

$$\int_0^d p'(z)dz = 1$$

which can be obtained by renormalizing the probability P(t) with respect to P(d):

$$\xi = \frac{P(t)}{P(d)} = \int_0^t \frac{p(z)}{P(d)}dz = \frac{\mu}{\omega_{0z}P(d)}\int_0^t exp\left[-\frac{\mu z}{\omega_{0z}}\right]dz = \frac{1 - exp\left[-\frac{\mu t}{\omega_{0z}}\right]}{1 - exp\left[-\frac{\mu d}{\omega_{0z}}\right]}$$

From this last equation it is obtained the position at which occurs the first **forced** collision

$$t = -\frac{\omega_{0z}}{\mu} ln(1 - \xi P(d))$$

## 2.4. Full transport equation: addition of the scattering term

The full transport equation for a a source of photons, monochromatic and monodirectional, in 1-D is given by

$$\omega_z \frac{\partial f}{\partial z} = -\mu f + \int_{4\pi} d\vec{\omega}' \int_0^{\infty} d\lambda' f(z, \omega', \lambda') k(\omega, \lambda, \omega', \lambda') + I_0 \delta(\vec{\omega} - \vec{\omega}_0) \delta(\lambda - \lambda_0) \delta(z)$$

where $k(\omega, \lambda, \omega', \lambda')$ represents the scattering kernel which changes the state of photons from $(\vec{\omega}', \lambda')$ to $(\vec{\omega}, \lambda)$.

(Note: it is always considered a particle without charge in order to exclude the action of long distance fields)

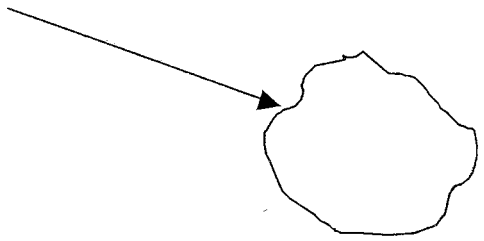
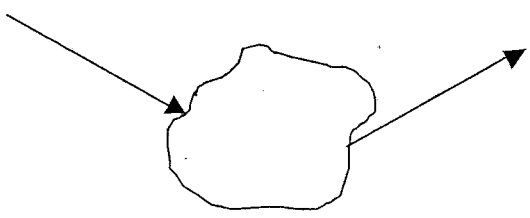
Let us consider the total probability of scattering $\sigma/\mu$ to undergone a collision which changes the state of the photon without absorbing it.
The scattering coefficient $\sigma$ is defined as

$$\sigma(\vec{\omega}', \lambda') = \int_{4\pi} d\vec{\omega} \int_0^{\infty} d\lambda \; k(\vec{\omega}, \lambda, \vec{\omega}', \lambda')$$

In similar way, the probability of absorption reduces to

$$\frac{\mu - \sigma}{\mu} = 1 - \frac{\sigma}{\mu}$$

It is clear that thanks to the scattering term we can (and we should) take into account another collisions after the first one. Let us see why, by observing a collision:

| | |
|---|---|
|  Fig 2a. Absorption collision | When there is only absorption, it is produced just attenuation of the beam |
|  Fig 2b. Scattering collision | When there is scattering, the particle is not lost but it remains, changing its state in the phase space (i.e., E' $\rightarrow$ E; $\vec{\omega}' \rightarrow \vec{\omega}$) |

How we consider the changes of state produced by the collision? → by considering the interaction kernel to generate the new state

For instance, for a kernel whose angular distribution has azimuthal symmetry, to obtain the scattering angle $\theta$ ($cos\,\theta = \bar{\omega}\cdot\bar{\omega}'$) we use the distribution function

$$p_\theta(cos(\vartheta),\lambda') = \frac{2\pi}{\sigma}\int_0^\infty d\lambda\ k(\bar{\omega}\cdot\bar{\omega}',\lambda,\lambda')$$

The azimuthal angle is obtained, in turn, from an even distribution in the interval $[0, 2\pi)$,

$$\varphi = 2\pi\xi$$

For a general kernel whose angular distribution has not azimuthal symmetry, to obtain the scattering angle $\theta$ ($cos\,\theta = \bar{\omega}\cdot\bar{\omega}'$) we use the distribution function

$$p_\theta(cos(\vartheta),\lambda') = \frac{1}{\sigma}\int_0^{2\pi} d\varphi\int_0^\infty d\lambda\ k(\bar{\omega},\lambda,\bar{\omega}',\lambda')$$

Once determined the value of $\theta$, it can be substituted in to the distribution function for $\varphi$

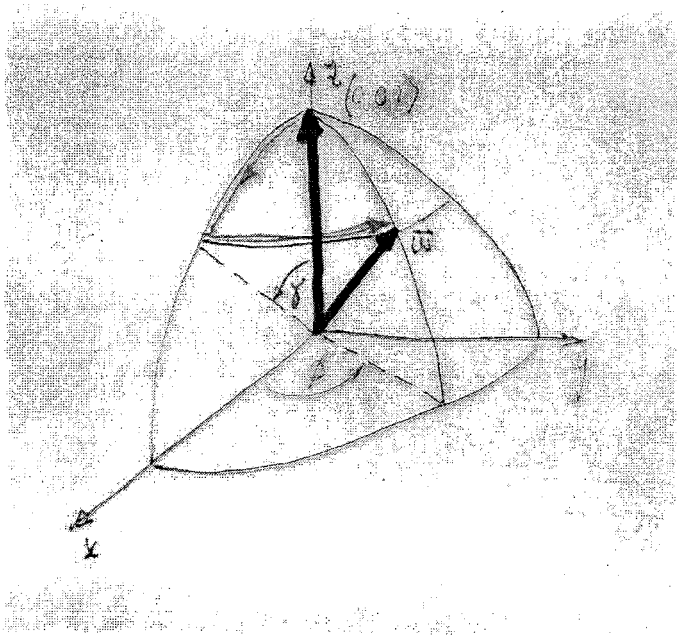
$$p_\varphi(,\lambda') = \frac{1}{\sigma}\int_0^\infty d\lambda\ k(\bar{\omega},\lambda,\bar{\omega}',\lambda')$$

**Warning: the description of the interaction takes place in the system CM (centre of mass) while the transport takes place in the Laboratory system**

Conventionally, in the system CM we consider $\bar{\omega}'\cdot\hat{z} = 1$

Standard calculation procedure:

1) The propagation vector is transformed form the Laboratory system to the CM system (i.e., the direction $\bar{\omega}'$ which has an arbitrary orientation in the space, is transformed to the $\hat{z}$ direction).
   This transformation is made in the following way: to bring the point (0,0,1) on the point $\bar{\omega}'$ two rotations are necessary: the first one around the y-axis by an angle $\gamma$, and the second one around the z-axis (obtained after the first rotation) by an angle $\phi$ (see figure).



| | | |
|---|---|---|
| Compton Scattering | $\frac{E_0}{1+\frac{E_0}{m_e c^2}(1-\cos\theta)}$ | Anisotropic<br>Heavily privileged the "backward" direction, i.e. with angle $\Theta=180^\circ$. |
| photoelectric "Scattering" | Characteristic energies $E_i$ | Isotropic |

A comparison with deterministic calculations (performed by separating the orders of collisions) shows that:

certain particular situations deserve special methods to be simulated efficiently (for instance, the extreme of the double Compton collision, see figure 4)

it has the advantage of allowing the computation of the higher collision orders, which are not easily computable with deterministic methods

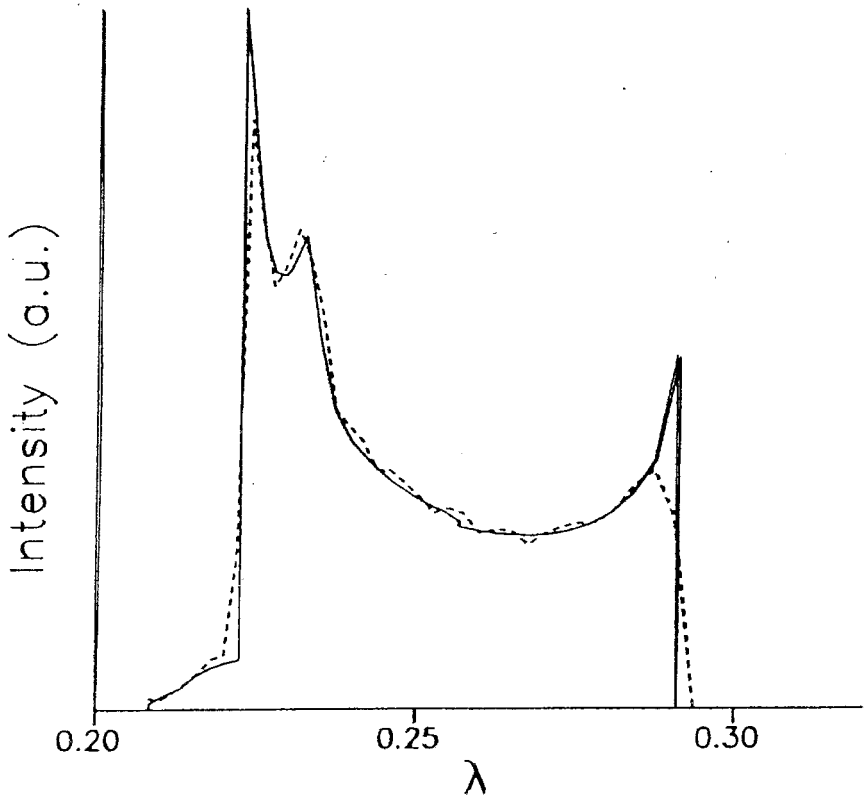



Figure 3. Example of disagreement between Monte Carlo and deterministic computations in some special regions which are particularly difficult to simulate. Is apparent the difference in the extremes of the double Compton distribution.

Clearly, the inverse rotation is used to bring back $\vec{\omega}'$ on the direction $\hat{z}$.

The resulting rotation follows:

$$A^{-1} = \begin{pmatrix} \frac{uw}{\rho} & \frac{vw}{\rho} & -\rho \\ \frac{-v}{\rho} & \frac{u}{\rho} & 0 \\ u & v & w \end{pmatrix}, \text{ with } \rho = \sqrt{1-w^2},$$

makes possible the transformation

$$A^{-1}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

2) The change of state for the given interaction is calculated (including the variation in the direction of the propagation vector)
3) The new propagation vector is transformed back to the Laboratory system

This procedure can be simplified by omitting the step 1, and by modifying the step 3:

4) The change of state for the given interaction is calculated (including the variation in the direction of the propagation vector)
2) The computed variation for the propagation vector is transformed (back) to the Laboratory system, and is vectorially added to the propagation vector before the interaction

**As a further complication different types of scattering can be considered: $\sigma_1$, $\sigma_2$, $\sigma_3$,...** $(\sigma = \sigma_1 + \sigma_2 + \sigma_3 + ...)$.

In this case, each type of scattering will be treated separately.

The above expression indicates that these are <u>independent</u> and <u>mutually excluding</u> events, and therefore, should be treated independently.
The random choice of the event ***k*** is made depending on the interval to which the random number $\xi$ belongs

$$\frac{\sigma_1}{\sigma} + ... + \frac{\sigma_{k-1}}{\sigma} \le \xi < \frac{\sigma_1}{\sigma} + ... + \frac{\sigma_k}{\sigma}$$

The choice of the type of event determinates the rules for the computation of the new state of the photon by using the kernel corresponding to the chosen interaction ***k***.

Example: photon transport with energy $E_0$ lower than 1 MeV (three types of possible interactions)

| Interaction type | Energy of the photon after the collision | Propagation direction after the collision |
|---|---|---|
| Rayleigh Scattering | $E_0$ | Anisotropic<br>Heavily privileged the "forward" direction, i.e. with scattering angle $\Theta=0^\circ$. |

**Another problems, more complexes, which require special techniques:**

- Zone transitions (i.e. when the particle passes from one region with masic absorption coefficient k to another with coefficient j),
- When there are different types of particles involved in the transport (coupled transport equations),
- Charged particles (long distance fields require special techniques to treat the continuous scattering),
- Wave effects (can be described partially using a vector equation for the transport, and similarly a "vector" Montc Carlo which uses 4 accumulators and not 1).
- Special direction effects (small scattering, coherence, molecular scattering, etc.)