Time improvement of photoelectric effect calculation for absorbed dose estimation

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Abstract. Ionizing radiation therapy is a very useful tool in cancer treatment. It is very important to determine absorbed dose in human tissue to accomplish an effective treatment. A mathematical model based on affected areas is the most suitable tool to estimate the absorbed dose. Lately, Monte Carlo based techniques have become the most reliable, but they are time expensive. Absorbed dose calculating programs using different strategies have to choose between estimation quality and calculating time. This paper describes an optimized method for the photoelectron polar angle calculation in photoelectric effect, which is significant to estimate deposited energy in human tissue. In the case studies, time cost reduction nearly reached 86%, meaning that the time needed to do the calculation is approximately 1/7 th of the non optimized approach. This has been done keeping precision invariant. Keywords: Optimization, Monte Carlo, Radiotherapy.

1. Introduction
Calculation of the energy deposited in matter by ionizing radiation (X and Gamma radiation, electrons, Alpha particles, etc.) is of interest in different areas, in particular in medicine.

The energy deposited per mass unit is called dose (D). Dose distributions in tissue brought about by photons are calculated in cases such as x-ray pictures, axial computed tomography and oncology treatments with ionizing radiation. Due to the large energy deposited in tissue by ionizing radiation in radiotherapy, dose distribution calculation is of paramount importance.

Four different interactions may occur between electromagnetic radiation with matter for the energy values used in radiotherapy: coherent interaction (Rayleigh), incoherent interaction (Compton), photoelectric effect and pair production [1].
Photon and particle interactions with a media are random phenomena which can be described by means of occurrence probabilities. The free path of a particle before interaction and the emerging energy and angles of the trajectory of the resulting particles have been modeled with equations that link them to occurrence probabilities of the different kinds of interactions. Manipulating those equations in such a way to calculate cumulative probabilities, allows to numerically simulation of the history of a particle by means of a sampling random numbers procedure (called Monte Carlo method). The first interaction of a particle (photon or electron) with a media and the interaction of the resulting particles and their trajectories will be referred to as the history of the initial particle. When the net effect over the media of a large number of histories is compiled, an estimation of the distribution of the energy deposited on the media is obtained. It is unavoidable to model a truly large number of histories to obtain results consistent with actual irradiation procedures. Many of the existing strategies based on the Monte Carlo method use what is known as the reject function to obtain so called “valid” results from the point of view of the problem. These reject functions use several random numbers increasing the calculation time [2].

The importance of fast calculation of the energy deposited in a given volume in the patient can be easily seen since oncology treatment planning is done using a trial and error approach. Every try consists of a possible configuration (flux of photons and their spectral composition, distance, energy and incident angles) for which the deposited energy is calculated and compared against desired values. Radiation treatments usually consist in evaluating the dose distribution for different configurations of beams, which lead to an increase of the computational time.

The macroscopic net effect of ionizing radiation is to modify the molecular structure of cells. When this happens, cells viability is affected. It is believed that genetic DNA of the cell nucleus is the critical target for ionizing radiation in cancer treatment.

The basis for radiotherapy is that cancer cells are more sensitive to ionizing radiation than normal cells. This has been extensively proven by means of the observation of tissue responses [3].

This paper introduces a strategy to reduce the calculation time of the photoelectric interactions while preserving precision, reviewing the construction of the cumulative density probability of the phenomenon. Section 2 presents basic aspects of the photoelectric effect and a classical strategy for full physics history calculation using Monte Carlo approach. Section 3 describes the proposed improvement, while section 4 depicts experimental data collected using both algorithms. Conclusions and future works are presented in section 5.

2. Photoelectric effect

During photoelectric interaction of photons with matter, a photon of energy $E$ is absorbed by a target atom which passes to an excited state emitting an electron (called photoelectron) with energy $E_e$ and polar angle $\theta_e$. Figure 1 shows a scheme of photoelectric interaction.

![Photoelectric effect](image)

Figure 1: Photoelectric effect

The photon beams found in radiation transport studies have relatively low photon densities and, as a consequence, only single-photon per atom absorption is observed.
To represent the atomic states we can adopt an independent electron model, such as the Dirac-Hartree-Fock-Slater [4] self-consistent model in which each electron occupies a single-particle orbital, with well defined ionization energy. The set of orbitals with the same principal and total angular momentum quantum numbers and the same parity constitute a shell. Each shell “i” can accommodate a finite number of electrons, with characteristic ionization energy \( U_i \). Notice that the shell ionization energies are positive; the quantity \( U_i \) represents the “binding” energy of each individual electron [2].

The trajectory of the emitted electron in relation with that of the absorbed photon is defined by means of both polar (\( \theta_e \)) and azimuthal (\( \phi_e \)) angles. Assuming that incident photon is not polarized, the photoelectron distributions is independent from the azimuthal angle, meaning that they are equally distributed among 0 and 2\( \pi \). The polar angle is obtained from the cross sections for the K-shell obtained by Sauter [5]. Equation (1) shows the expression of the differential cross section per electron (\( \sigma_{ph} \)).

The Sauter Differential Cross Section DCS (per electron) can be written as:

\[
\frac{d\sigma_{ph}}{d\Omega_e} = \alpha^4 r_e^2 \left( \frac{Z}{k} \right)^5 \frac{\beta^3 \sin^2 \theta_e}{\gamma (1 - \beta \cos \theta_e)} \Gamma^* \left[ 1 + \frac{1}{2} \gamma (\gamma - 1)(\gamma - 2)(1 - \beta \cos \theta_e) \right]
\]

where \( \alpha \) is the fine structure constant, \( \gamma = 1 + \frac{E_e}{m_e c^2} \), \( \beta = \frac{E_e (E_e + 2m_e c^2)}{E_e + m_e c^2} \), \( E_e \) the photoelectron energy, \( r_e \) is classical electron radius, \( m_e \) the electron mass and \( c \) the light speed.

2.1. Relative relevance of different interactions of X and Gamma radiation with tissue.
When a beam of photons passes through an object, some photons will be transmitted through the material without interaction. There is an exponential relationship between the number of incident photons (\( N_0 \)) and those transmitted through thickness \( d \) without interaction. The relationship is expressed in equation (2), where \( d \) is the total thickness of the material, \( N \) is the number of photons which emerge from the slab without having interacted, \( \rho \) is the material density and \( N_0 \) is the number of photons entering the slab [6].

\[
N = N_0 e^{-\sum \frac{\mu_i d}{\rho}}
\]

The interaction type that takes place between radiation and matter depends on the incident photon energy and the kind of interacting material. Figure 2 shows the coefficients of mass attenuation for photons in water.

In the cases of X-Ray pictures and Axial Computed Tomography, energies lower than 100 KeV are used and thus photoelectric interaction is predominant over Compton and Rayleigh.

Most of the energies of photons in Radiotherapy are higher than 1 Mev. Even though Compton and Pair production are predominant at these energies, successive interactions will produce photons with lower energies that will interact more likely by photoelectric effect. Additionally to the photons with energies higher than 1 MeV, LINACs emit photons with energies as low as 10 KeVs. According to figure 2, the photoelectric effect becomes more important.

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Therefore, photoelectric interaction must also be taken into account when a flux of high energies photons (> 1 MeV) is used.

Figure 2: Photon Mass absorption coefficients for different interactions

2.2. Random Numbers Quality
Monte Carlo based methods consume large quantity of random numbers; in addition they must accomplish certain quality requirements.

Most frequently, simulations are based on pseudorandom numbers because their generation is computationally suitable. Algorithms for truly random numbers generation are unacceptable for calculation since they are computationally expensive. Then, they are usually taken from a previously calculated table.

Truly random numbers such as the π number digits does not require any verification; however pseudorandom numbers must meet some properties before their use in any Monte Carlo calculation. Most adequate test to ensure such properties are: frequency test of every digit, pokers hand testing (comparison between the expected and obtained value of a given combination of digits), serialization test to find any possible association between digits [7]. As it will be detailed ahead, every calculation done in this work has been done with fully tested random numbers.

2.3. Monte Carlo method with reject function
In what follows, the use of the rejection method for photoelectric interaction is briefly described.

2.3.1. Azimuthal angle calculation.
Since the azimuthal angle is equally distributed between 0 and 2π, its sampling may be done using equation 3, where ξ₀ is a random number equally distributed between 0 and 1.

\[ \Phi = \xi_0 \times 2 \pi \]  

2.3.2. Electron energy calculation.
The emitted electron kinetic energy is obtained by subtracting the ionization energy \( U_i \) from the arriving photon energy (see Equation 4).

\[ E_e = E - U_i \]  

2.3.3. Electron polar angle calculation.
In this subsection a classic polar angle calculation method using a Monte Carlo based technique with reject function is described.
Introducing $\nu = 1 - \cos \theta$, angular distribution of photoelectrons can be expressed (leaving a normalization constant) in the form shown in equation (5).

$$p(\nu) = (2 - \nu) \frac{1}{A + \nu} + \frac{1}{2} \beta \gamma (\gamma - 1)(\gamma - 2) \frac{\nu}{(A + \nu)^3}$$

with $A = \beta^2 - 1$.

Random sampling of $\nu$ may be accomplished by means of:

$$p(\nu) = g(\nu) \pi(\nu)$$

$$g(\nu) = (2 - \nu) \left[ \frac{1}{A + \nu} + Q \right]$$

$$\pi(\nu) = \frac{A(A + 2)^2}{2} \frac{\nu}{(A + \nu)^3}$$

The variable $\nu$ takes values within the interval $[0;2]$. The function $g(\nu)$ is definite positive, attains its maximum value at $\nu = 0$, and its monotonically decreasing while the function $\pi(\nu)$ is positive and it is normalized to unity. Taking $\pi(\nu)$ as a probability density function, sampling random values of it may be generated by means of a random number $\xi$ and solving equation 9, which may be done analytically, leading to equation 10.

$$\int_0^\nu \pi(\nu') d\nu' = \xi$$

$$\nu = \frac{2A}{(A + 2)^2 - 4\xi} \left[ 2\xi + (A + 2)\xi^{1/2} \right]$$

Therefore, random sampling from Sauter’s distribution can be performed by the rejection method as follows:

i) Sample a random number $\xi_1$

ii) Calculate $\nu_1$ using equation (10) and $\xi_1$.

iii) Sample a random number $\xi_2$

iv) If $\xi_2 g(0) > g(\nu_1)$ return to step i)

v) If $\xi_2 g(0) \leq g(\nu_1)$ then use $\nu_1$ to calculate $\theta$.

The previous algorithm fits in the classic model for Monte Carlo based strategy using the inverse of the cumulative probability density function (Equation 9) combined with a reject function. Step iv) is a reject function and requires at least one extra random number $\xi_2$ for verification purpose. Depending on the number of rejections this procedure requires 2, 4, 6, or even more random numbers to calculate a single polar angle, which increases computational times.

The average wall time needed to calculate $1*10^6$ valid angles is about 2.5 seconds using a C language program running on a 3.2 Ghz, 800 MHz Front Serial Bus, Pentium IV computer.

The number of random numbers required to calculate $1*10^6$ angles varies from $5*10^6$ to $7*10^6$ for energies where the photoelectric effect is predominant, then an average of 5 to 7 random number are used for every polar angle.

Figure 3 shows angle distribution obtained for $1*10^4$ incident photons with 10 KeV energy. Ten $\pi/5$ intervals were used.
3. Suggested method

The proposed method replaces the Monte Carlo algorithm with reject function by another Monte Carlo algorithm which embeds the reject function within the cumulative density probability function [8]. In other words, it does not proceed with the factorization of equation (5) into equation (6) but calculates \( \nu \) integrating equation (5). Integrating the probability density function analytically, equation 11 is obtained.

\[
\int_0^\infty \nu \cdot p(\nu) d\nu = \frac{(A^2 + 2A)}{3(A + \nu)^3} \cdot \left( A + \frac{1}{2} QA - \frac{1}{2} QA^2 \right) - \frac{(2Q + 2QA - 1)}{(A + \nu)} \cdot Q \ln(A + \nu)
\]

(11)

Figure 4 depicts the values given by equation (10) for incident photons with energy of 10 KeV.

3.1. Implementation

Equation (11) requires just one random number to calculate the polar angle. This fact reduces the computation overall time, however, further improvements may be accomplished considering that the equation mentioned may be fully pre-calculated. A cross table, having energy in columns and cumulative probability in rows was built [8].

The cross table contains emerging photon polar angles. Then, a simple bilinear interpolation allows obtaining \( \theta_e \) values for each random number sampled.

By performing a sensibility test on the results obtained by the bilinear interpolation it was found out that there is a small portion of the table which provides results with excessive error. These errors may be reduced by means of bi-cubical interpolation. However, the increase in computation time discourages this solution. On the other hand, enlarging the table by reducing the step in rows and or...
columns will far increase the program size. As a compromise among precision, size and computation time, the table was split in two. First, one for low energies where the error is larger, and a second one for higher energies where the interpolation error may be neglected.

4. Experimental results
Comparing overall calculation time of Monte Carlo based algorithm with a reject function against table based Monte Carlo algorithm, a very important difference was found. An average of 23.8 seconds was required to calculate $1 \times 10^7$ angles with the reject method, while the improved tabled based algorithm only needed 3.2 seconds. Both fragments of code were written in C, and they were run on a 3.2 Ghz, 800 MHz Front Serial Bus, Pentium IV computer.

5. Conclusions and future work
In this paper an algorithm to perform Monte Carlo calculation to determine the polar angle of the emitted photoelectron has been presented. It shortens the overall computation time by seven.

It is planned to apply the same strategy to the calculation of angles and energies of the electron and secondary photon of the Compton Effect since the rejection function is also employed in Compton interaction calculations. Preliminary studies lead to estimate that the potential reduction in the quantity of random numbers required in the overall computation time may be similar to or even greater than the one obtained for the photoelectric effect [9].

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