A REVIEW OF MONTE CARLO METHODS AND THEIR APPLICATION IN MEDICAL PHYSICS FOR SIMULATING RADIATION TRANSPORT

[1]*Safarov Abror*, [1]*Mukhammedov Umidjon*, [1]*Ashurov Sindorjon*
[1]*National University of Uzbekistan named after Mirzo Ulugbek*
sindorphy@gmail.com

Abstract

Monte Carlo methods are used to calculate statistical behavior through the use of random number generators and probability density functions. They have been used extensively in medical physics for research in radiotherapy, designing technology, dosimetry, and advanced clinical applications. This paper provides a background on Monte Carlo methods and a review of radiation therapy physics and dosimetry. Additionally, there is a discussion of the different ways Monte Carlo methods are used in medical physics as well as a review of current research related to Monte Carlo methods. The final portion of this paper contains my own Monte Carlo simulation using the EGSnrc software toolkit to carry out two different simulations. One simulation serves as a basic introduction to using the software and demonstrates some of its capabilities, while the other is a more complex simulation that models a realistic scenario in medical physics.

Keywords: Monte Carlo, medical physics, radiation transport, EGSnrc, simulation, dose, random numbers

Introduction

The Monte Carlo (MC) method is a widely used technique with a variety of applications. It can be difficult to provide an exact definition for MC methods due their diversity in application, therefore for our purposes it will be defined in the general context of medical physics as the following: Monte Carlo is a numerical method to solve equations or to calculate integrals based on random number sampling [1].

Random number generators (RNG) are required for a MC simulation in order to produce a large set of uncorrelated numbers. Since computer program outputs are inherently predictable, they must appear random. Therefore the result of these RNGs must be “pseudorandom”. A useful RNG for applications in radiation therapy must have the following
attributes.

• Have a period long enough such that it is not used several times, making the results of the MC simulation correlated.

• The numbers must be uniformly distributed in multiple dimensions. More specifically, random vectors of n-tuple random numbers must be uniformly distributed in n-dimensional space.

One class of simple RNGs is the linear congruential generators which produces a sequence of integers In by the recurrence relationship

$$I_{j+1} = (aI_j + c) \bmod m \qquad (1)$$

where a is a multiplier, c is an increment, and m is a modulus. The CERN program library is a good resource for finding high-quality RNGs and test programs to observe the created sequences in multiple dimensions [2].

The MC method can be used as a stochastic method for numerical integration which is capable of solving equations that would otherwise be impossible analytically [2]. Consider an area A enclosed by the function f (x) on the interval [a, b].

$$A = \int_a^b f(x)dx$$

Then a randomly generated number ηi uniformly distributed in the range [0,1] can be scaled to the range [a, b] by

$$\xi_i = (b-a)\eta_i + a$$

thus ξ_i is uniformly distributed in the range [a, b]. Then we can give a rough estimate of the area A by

$$A_1 = (b-a)f(\xi_1)$$

then repeating and improving this estimate by averaging the areas from two runs

$$A_2 = \frac{1}{2}[(b-a)f(\xi_2) + A_1] = \frac{b-a}{2}[f(\xi_1) + f(\xi_2)] \qquad (2)$$

Therefore the generalization becomes obvious after continuously repeating this process.

$$A_N = \frac{b-a}{N}\sum_{i=1}^{N} f(\xi_i) \qquad (3)$$

In the limit N →∞, the estimated area A_N converges to the real integral A. This method can be expanded to multiple dimensions. Assume f (x) is now a function that shall be integrated in a volume V with D dimensions. Now instead of random numbers for the MC integration, we need a set of random points (or vectors) uniformly distributed in the multidimensional volume V. If we have our randomly generated set $\xi_1 \ldots \xi_N$, then this leads us to the basic theorem of MC integration which includes the uncertainty of the estimation

$$\int dVf(x) \approx V < f(x) > \pm (b-a)\sqrt{\frac{<f^2(x)> - <f(x)>^2}{N}} \qquad (4)$$

where Eq.(5) is the average function value and average function value squared respectively[4].

$$< f(x) >= \frac{1}{N}\sum_{i=1}^{N} f(\xi_i) \quad \text{and} < f^2(x) >= \frac{1}{N}\sum_{i=1}^{N} f^2(\xi_i) \qquad (5)$$

Review of Radiation Therapy Physics and Dosimetry

Radiation therapy uses ionizing radiation to harm and destroy cancer cells. Ionization is the process of a neutral atom either gaining or losing an electron, becoming a negatively or positively charged ion respectively. When charged particles such as protons, electrons, and α particles have a sufficient amount of kinetic energy capable of ionizing a neutral atom through collisions, they are known as directly ionizing radiation. Alternatively, neutral particles such as neutrons and photons capable of ionization are known as indirectly ionizing radiation [8].

The four primary processes responsible for ionization in radiotherapy are the Compton effect, photoelectric effect, coherent scattering, and pair production[5].

It is important to define the characteristics of the beam emitting x-rays or γ-rays from a radioactive source. These beams contain a large number of photons in a variety of energies [6]. The fluence (Φ) of a beam, which has units of m^{-2} , is analogous to flux in electromagnetism. It is defined as the number of photons (dN) that enter a cross-sectional area (da)

$$\Phi = \frac{dN}{da} \qquad (6)$$

Then naturally the fluence rate (φ), also known as flux density, is defined as the fluence per unit time.

$$\varphi = \frac{d\Phi}{dt} \qquad (7)$$

Radiation dosimetry deals with methods for quantitative determination of energy deposited in a medium through direct or indirect ionizing radiation [7]. A variety of quantities and key calculations will be defined in this section. Kerma, which stands for kinetic energy released per unit mass, is a non-stochastic quantity that is applicable for indirectly ionizing radiation such as photons and neutrons. It represents the energy transferred from indirectly ionizing radiation to the charged particles. It can be defined quantitatively as

$$K = \Psi(\frac{\mu_{en}}{\rho}) /(1 - \underline{g}) \qquad (8)$$

where μ_{en}/ρ is the averaged mass-energy absorption coefficient and $\bar{g}$ is the average fraction of an electron energy lost to radiative processes [8]. Kerma has units of J/kg or, in SI units, Gray (Gy). Kerma can also be divided into two components; inelastic collisions with atomic electrons (K^{col}) and radiative collisions with atomic nuclei (K^{rad}). Therefore Kerma can be written as a sum.

$$K = K^{col} + K^{rad} \qquad (9)$$

Similarly cema, which stands for converted energy per unit mass, is a non-stochastic quantity that is applicable for directly ionizing radiation such as electrons and protons. It represents the energy lost by charged particles (dE_c) in a unit of mass

(dm) of material. It can be described quantitatively by Eq. (10) and it has the same units as Kerma.

$$c = \frac{dE_c}{dm} \qquad (10)$$

Absorbed dose (D) is applicable to both indirectly and directly ionizing radiation and can be defined as the mean energy ($\bar{\varepsilon}$) imparted by ionizing radiation to matter of mass m. The absorbed dose is often usually derived from energy loss along a particle path-length segment, thus it's related to particle fluence. It's common to calculate the fluence differential in energy (Φ_E), which has units cm^{-2} MeV^{-1} [1]. When calculated through MC simulations, for either charged or uncharged particles, the absorbed dose in the medium (D_{med}) can be calculated by the following equations.

$$(D_{med})_{CPE} = \int_0^{E_{max}} [\Phi_E]_{med}[S_{el}(E)/\rho]_{med}dE \quad \text{for charged particles} \qquad (11)$$

$$(D_{med})_{TCPE} = \int_0^{k_{max}} k[\Phi_k]_{med}[\mu_{en}(k)/\rho]_{med}dk \quad \text{for photons} \qquad (12)$$

Eq(11) and Eq(12) can also be used to calculate the absorbed dose in a detector (D_{det}). The acronyms over the equal signs CPE and TCPE stand for charge-particle equilibrium and transient charged-particle equilibrium respectively. Charged-particle equilibrium exists for a volume V if each charged particle of a given type and energy leaving the volume is replaced by an identical particle entering [12]. This is for lower energy particles, typically below 500 keV, since attenuation can be neglected. If there is no CPE then the quantity calculated in Eq. (11) is not absorbed dose, instead it is cema (C). Transient charged-particle equilibrium occurs for higher energy particles since attenuation causes there to be less charged particles produced with increased depth [7]. If there is no TCPE then the quantity calculated is kerma (K). Additionally it is important to note k as the photon energy and S_{el}/ρ as the mass electronic stopping power (additional info can be found in ICRU Report 85 [1]).

Using Eq (11) and Eq (12), the Bragg-Gray stopping power ratio can be defined as

$$S^{BG}{}_{med,det} = \frac{\int_0^{E_{max}} [\Phi_E]_{med}[S_{el}(E)/\rho]_{med}dE}{\int_0^{E_{max}} [\Phi_E]_{med}[S_{el}(E)/\rho]_{det}dE} \qquad (13)$$

where we use the Bragg-Gray assumption which says that the cavity (detector) is so small that it does not disturb the fluence of the charged particles when inserted into the medium [5]. This gives us the condition $\Phi_{med} \approx \Phi_{det}$. It is also assumed that the primary charged-particle fluence does not include secondary or higher-order particles produced by collisions with the primary particles.

Monte Carlo Methods in Medical Physics

Monte Carlo methods help both clinical physicists and researchers in better understanding dose calculations and modeling a variety of radiation sources. This section explores the use of Monte Carlo methods in dosimetry, external beam source modeling, and for advanced treatment planning.

When determining dose calculations experimentally, there are often quantities that are difficult or even impossible to calculate analytically. Therefore these quantities need to be determined numerically through the use of MC methods. In radiation dosimetry, detectors are typically composed of several different components. The materials of each of these components differ substantially from the medium where the absorbed dose is to be determined [8]. This leads to a well established problem that is characterized in terms of perturbation factors. Inserting a detector in a medium causes a change in the electron spectrum within the detector radiation sensitive volume relative to that in the homogeneous medium. This effect is known as perturbation [1]. Now taking into account these perturbation factors, and assuming the Bragg-Gray assumption is valid, the absorbed dose of the medium becomes

$$D_{med} = \underline{D_{det}} \cdot s_{med,det}(Q) \cdot p_{det}(Q) \qquad (14)$$

where $p_{det}(Q)$ is the perturbation factor of the detector and Q is a given radiation beam quality. A major constraint imposed on the perturbation factors is that they are small and independent of each other.

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