Monte Carlo Method and Their Codes Applied to Ionizing Radiation

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Abstract. The Monte Carlo method is a tool of high importance in the contemporaneous context. Not only does its statistical approach allow estimating integrals and differentials equations that do not have an analytical solution, as it also allows that events of stochastic nature can be simulated. In this context, it will be explored the use of the method in the universe of ionizing radiation as a foundation of a project looking for the implementation of a metrology 4.0. In this sense, the following codes will be explored: GEANT4, EGSnrc, PENELOPE and MCNP exhibiting vantages and disadvantages concerning their use.

1. Introduction

In general, the name Monte Carlo (MC) method comes from similar functioning casino games. It is any statistical method that is a big random sampling based through specific techniques with repeated simulations looking for probability distribution obtained. This method is largely used in physics, biology, chemistry, mathematics allowing functions statistical solutions which do not have experimental data. In this sense, it could be satisfactorily defined as a statistical approach to problems without an analytical solution due to stochastic nature of the phenomena, or because of a big amount of freedom degrees that the physical system possesses.

This statistical tool comes up as a third strand for approaching the nature, diverging from the experimental and theoretical physics bipolarity, that is still strong in current days. In this context, the MC is a vital tool in experiments that have a high cost, limiting the experimentation. This sentence is illustrated in the nuclear field development that would be very expensive to test the efficiency of the devices in experiments, making the simulation a high importance tool.

Although this example might seem related to the middle of the XX century, the human journey in cosmos faces complex troubles that this statistical approach would play a role of high relevance. The simulation, in this context, can be used as a vital part in planning and estimating the effective dose aiming the astronauts radioprotection in lunar, Martian soil and in the stay in Deep Space Gateway.

However, before getting in the contemporaneous use of the method in ionizing radiation physics, is necessary to understand MC formulation. Essentially, in a great number of the research group, four vital
researchers stand out in the MC method. Stanislaw Ulam and John Von Neumann for the method concept and also Klara Von Neumann and Nicholas Metropolis for the protagonist in the code construction to run on ENIAC (Electronic Numerical Integrator and Computer) in the modern code paradigm. It is worth mentioning that this history advanced, is not exclusively on the first MC method running in an electronic computer, but also the first code in history to run in the modern code paradigm.

2. The Beginning of The Method
The MC method comes up in the historical context in the second world war final intending to give information that results in geometries and methods for the construction of more efficiently nuclear weapons before detonating this device and verify in that way their efficiency and viability. It is estimated that only 1% of the 64 kg of Hiroshima bomb uranium suffered fission. In this context, it is reasonable to imagine that MC acting in geometry and materials simulation applied in a nuclear device would be capable of increasing the bomb efficiency that Hiroshima had without making countless experimental tests.

However, the method history initiates even before it possess name. Henrico Fermi, in Rome, 15 years before Nicholas Metropolis suggest the name to the method, did simulations in his works that were capable of giving good experimental predictions. In the paper “The beginning of Monte Carlo method” [2] recognize what Fermi did quoting the student and collaborator of the Italian physicist.

“Fermi had invented, but of course not named, the present Monte Carlo method when he was studying the moderation of neutrons in Rome. He did not publish anything on the subject, but he used the method to solve many problems with whatever calculating facilities he had, chiefly a small mechanical adding machine.”

Observing these facts, it is inconceivable not to question why it takes 15 years for the formal approach of MC in researches. In relation to this question, it is necessary to go further in the method structure that passed through the building of the first electronic computer called ENIAC, by the Ballistic Research Laboratory in Aberdeen, United States, as a tool of optimizing solutions of differential equations rather than laborious manual methods.

2.1. The Protagonism of ENIAC in MC
Initially, the ENIAC solved mathematics calculus, as it was designated by the John Mauchly and Presper Eckert proposal, and eventually, their calculus showed off the construction viability of a thermonuclear weapon in 1946. In this context, Stanislaw Ulam in the front of the miraculous capability of the electronic computer observed the possibility of employing statistical sampling in physical simulations using ENIAC, without it, the calculus would take a long time and would be complex. This possibility of using statistical sampling was discussed in a letter addressed to John Von Neumann.

Note that without a demonstration of the ENIAC power, in the hydrogen bomb development context, the issue of the sampling technique used would not have been discussed because the technique had already existed, but the manual approach did not seem viable.

In this sense, posteriorly, John Von Neumann would send a letter in 1947 to Robert Richtmyer detailing the method applicability in the statistical approach to the fissionable materials in the neutron diffusion problem. The method described in the letter had proposed to follow every neutron in the trajectory and interaction with the spherical reactor made of fissionable material surrounded by a shell. The simplified algorithm behind the simulation is represented in figure 1.

The flow chart, figure 1, translates the mechanism main idea that was implemented to ENIAC run for the first time in 1948. However, must be questioned how this simple scheme was responsible for such an innovative tool. The answer to this question is the employment of sampling techniques, this issue will be discussed later in this paper, in every box of the flow chart as a mechanism of taking decisions of the interactions, positions, speeds and trajectories that the neutron will go through in the material. In a succinct way, the method idea was growing up to track the history of a neutron using random numbers to select the events of many interactions over the trajectory employing sampling techniques.
3. Pseudorandom Number Generator

The random number generator is the artifice employed for sampling in the code decision points. In this sense, it is the heart of the simulation and the quality in which it generates numbers is directly correlated to the quality of the simulation. In the universe of random numbers, there are essentially three different types of generators: random number generator, pseudorandom number generator, and quasi-random number generator. However, the pseudorandom number generator is the method massively employed in MC simulations because it is fast, reproducible and provides satisfactory results in statistical tests.

The nomenclature with the prefix pseudo occurs essentially because these numbers are generated by a specific algorithm. In the MC method, these numbers are computer generated. This, in a brief way of speaking, is just a beautiful and complex group of capacitors and other electronic devices that work following clear and well-defined instructions. In our technological development and knowledge stage, these instructions are written in programming languages such as Python, C++, Fortran, and others, that will give instructions for the machine to follow. Once it is necessary to instruct the machine to generate numbers, this procedure is not random, because it follows a specific logic and consequently it is inserted a deterministic choice.

So how can these pseudorandom numbers be generated and why can we treat them as random? Answering this question, inspired by Hammersley and Handscomb [1], the concern about the random number sequence must not be in their generation mechanism, actually, it must concern if it is correctly distributed. When thinking about random number generation it is expected to obtain a rectangular distribution in how each number generated possesses the same probability to be chosen and also the capability of creating a sequence of non-correlated numbers. Nascimento et al [11] brought a discussion in this topic about random numbers.

4. Sampling Techniques

If the pseudorandom number generator can be treated as this method’s foundation, the statistical sampling techniques would be the supports and give the macrostructure shape. The function of this
technique takes place in the interaction of generated numbers with the probability density function (PDF). In figure 1, the mentioned interaction would inform if in the simulation history the neutron will be absorbed, scattered or if it will provide fission of nuclei.

Therefore, the statistical sampling concept already exists before the ENIAC construction and because of its ability to handle mathematical operations that were proposed to use these techniques as a computational simulation tool.

In general, we can look to the point that the code takes decisions as the structure in figure 2:

![Elementary sampling technique structure.](image)

Figure 2: Elementary sampling technique structure. The number generated is divided once again by its divisor in the recurrence, m, to produce random numbers u that is $0 < u \leq 1$, and so these numbers are ready to be sampling techniques used.

There are plenty of statistical sampling techniques. Those techniques were discussed in letters exchanged between Stan Ulam and John Von Newmann when the MC has been built. In one of his letters, John flagged to Stan a new method created for him that would be the rejection technic in opposite to the method of inverse transformation, which apparently was under consideration at the beginning of the method [12]. This following text demonstrates the most elementary method of sampling techniques, the Inverse transformation technic.

### 4.1. Inverse Transformation Technique

This method consists in the following aspect. Given a random number $u$, normalizing it in a way that it fits in the interval $0 < u \leq 1$ and let $p(x)$ be a PDF. We have, in the case of the PDF a rectangular distribution:

$$u = \int_{a}^{x} p(x') dx' \quad p(x') = \frac{1}{b - a} ; \quad a \leq x \leq b$$  \hfill (1)

After integrating, we must find the inverse function, therefore we will have a value $x$ written as a function of the random number sampled.

$$u = \int_{a}^{x} \frac{1}{b - a} dx' = \frac{x - a}{b - a} \rightarrow x = a + u(b - a)$$  \hfill (2)

Evidently, this method requires that the function possess its inverse and be continuous in all domains. These restrictions are a barrier for some simulations with the physics process possesses a PDF that is not continuous or invertible.
5. Ionizing Radiation MC Codes
There are a variety of codes available for use. However, for this job, only four were observed, which are
the most commonly employed in ionizing radiation. The following are some of the peculiarities of each
one.

5.1 GEANT (Geometry and tracking)
The MC code GEANT is another great contribution of CERN (Conseil Européen pour la Recherche
Nucléaire) for the scientific community. This tool was created in 1974 looking for particles interaction
study in some high energy physics detectors. Because of this purpose, it is able to simulate a big diversity
of types of particles in a large energy range. It is possible to simulate from de physics that is the target
of this paper, photons and electrons, to neutrons, protons, alpha particles, neutrinos, muons, mesons,
ions and many others.

The version 10 of GEANT4 acts in an energy range from 0.025 eV to 1 PeV (energy available only
to muons. However, photons, leptons, hadrons and ions are capable to reach the energy of 100TeV)
acting in that way in many fields of the knowledge since cosmic rays to radiobiology.

In that sense, the low energy aspect of 0.025 eV to 10 MeV is where the great innovations of this
code occur, that is the extension GEANT-DNA. These tools do not only simulate the interaction of
radiation with the biological system at the cellular level and DNA level but also simulate the chemical
effects produced by the radiation, for instance, the formation of free radicals and biochemical reactions.

5.2 PENELOPE (Penetration and energy loss photons and electrons)
PENELOPE was developed in 1995 and distributed by NEA (Nuclear Energy Agency), an organization
with 33 participants countries encompassing North America, Asia-Pacific region and Europe. It was
developed by Francesc Salvat, Jose Maria Fernandez-Varea and Josep Sempau. The 2008 version acts
in a range of 50 eV to 1 GeV for photons, electrons and positrons.

5.3 MCNP (Monte Carlo N-particle)
MCNP was developed in 1977 and distributed by Los Alamos National Laboratory. The version
MCNP5 acts in an energy range from 1 keV to 100 GeV (energy possible to simulate photons). On the
other hand, the range of electrons and positrons energy varies from 1 keV to 1 GeV and neutrons act in
the range of 10~11 MeV to 100 MeV.

5.4 EGSnrc (Electron gamma shower)
EGSnrc is the result of an enhanced EGS version that was made in 1970 by SLAC (Stanford Linear
Accelerator Center) National Accelerator Laboratory. The enhanced version was created in 2000 and
distributed by NRC (National Research Council). The version EGSnrc is capable to simulate the
transport of photons, electrons and positrons in an energy range from 1 keV to 10 GeV.

6. Conclusion
According to Teixeira et al, Vilches et al and Archamboult et al [8, 9 and 10], comparing the simulation
results obtained from each one of the codes, it was found that the results mutually agree without
accentuated discrepancies. The small divergence that could be observed is due to the elementary
differences in the models of cross sections employed in each code. In that sense, the search for an MC
code that would be the best for ionizing radiation is still a vague idea, because each code uses a different
cross sections library and when the particle, energy and the experiment are changed, the code panorama
that produces the best results could considerably change. Therefore, it will be shown some relevant
aspects to take under consideration while choosing one of those codes. Some important structural aspects
to choose a code are listed in table 1.
Table 1. MCNP5, GEANT4, EGSnrc and PENELOPE codes structural aspects.

| Structural aspects                  | MCNP5 | GEANT4 | EGSnrc | PENELOPE |
|-------------------------------------|-------|--------|--------|----------|
| Windows, MacOS and Unix             | ✓     | ✓      | ✓      | ✓        |
| Language of the source code         | Fortran | C++ | C++ and Fortran | C++ |
| Free distribution                   | ✗     | ✓      | ✓      | ✗        |
| Open code                           | ✗     | ✓      | ✓      | ✓        |
| Knowledge of programming            | ✗     | ✓      | ✗      | ✗        |
| Possess geometry viewer             | ✓     | ✓      | ✓      | ✓        |

In that sense, MCNP5, PENELOPE and EGSnrc are easy tools to run simple applications, you just need to configure input files, for instance, the geometry and materials of the physical event without the need of deeply understand any programming language.

However, this need is a prerequisite if it is required more complex applications. In that context, the GEANT4 is the most delicate code, because it is necessary to go inside the code written in C++ to make alterations to define geometry and material. Another factor that contributes to the GEANT4 complexity is the fact that it possesses a large range of applicability and because of that there are many libraries from low energies to high energy physics. In other words, there is much information required to be understood before making simulations.

Another important factor to ponder in the analysis of the MC codes is the geometry viewer. In this topic the GEANT4 is the most advanced, providing the user many possible 3D viewer types that also have an attractive and interactive interface where the user can rotate and translate the geometry in a simple way with the mouse. It is worth mentioning that EGSnrc provides only one possibility of 3D viewer. On the other hand, PENELOPE and MCNP5 only provide 2D projections of the object.

In the innovation topic, the GEANT4 stand out providing the extension GEANT-DNA, already mentioned, and also there is the simulate physical phenomena functionality in distinct environmental conditions from de NTP. However, it cannot be simulated physical situations where the material is not in the solid, liquid or gas state.

The last consideration to be done is due to the numbers of publications of scientific papers of each code. In that sense, the codes that stand out are the GEANT4 and EGSnrc in the Physics in Medicine and Biology and in the Medical Physics. However, in Metrologia, the PENELOPE possesses a slight superiority in comparison to the other codes, while GEANT4 do not have a single paper published as can be seen in figure 3 and figure 4.
Figure 3: MCNP5, GEANT4, EGSnrc e PENELOPE codes publishing during the period 01/01/1992 to 14/06/2019 in the magazine Medical Physics.

Figure 4: Publishing that quotes the four codes, MCNP5, GEANT4, EGSnrc e PENELOPE targets of this work in the period of 01/01/1992 to 14/06/2019 in the magazine Medical Physics, Metrologia and Physics in Medicine and Biology.

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