"MetroMC" RESEARCH GROUP: COMPUTATIONAL PHYSICS IN IONIZING RADIATION METROLOGY

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Abstract. The aim of this work is to highlight the undisputable needs and the suitability of computational physics in ionizing radiation metrology. In this matter, a new young research group has been developed within the *Department of Radioisotopes and Radiation Metrology* (DRMR) from Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), Romania. The above-mentioned research group named "MetroMC" (Monte Carlo in Metrology) is marking the start point of its research activity, in this actual form, through this paper. For this purpose, a simple theoretical experiment has been performed in order to compare the results obtained by approaching the same problem by various Monte Carlo codes that are currently being used by the group members (MCNP, GEANT4, and EGSnrs).

Key words: "MetroMC", Monte Carlo, ionizing radiation metrology.

1. INTRODUCTION

In the last years, there has been a great deal of importance and interest in the application of numerical simulations in almost all scientific areas [1–5]. In this paper, we will refer in particular to the Monte Carlo methods which are frequently employed in the various fields of nuclear physics, as nuclear physics started to appear more and more on the highlights due to the most recent discoveries, new state-of-the-art research infrastructure and its cutting-edge applications.

In all the applications of nuclear physics, the precise measurements (the activity of a radionuclide, absorbed dose, particle flux, energy, etc.) are mandatory. In this matter, the ionizing radiation metrology research groups are constantly working on providing new and more precise and dedicated calibration methods. In the last years, even in the case of metrology which is conceptually the science of the measurement, the computational methods are being applied increasingly and the widely used MC codes started to be more refined and provide coherent results, no matter what the particular applications are [6–13].

To provide support to the international trend of using MC codes in ionizing radiation metrology, a new young research group (MetroMC) has been formed within the *Department of Radioisotopes and Radiation Metrology* (DRMR) from Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH). The institute is designated by INM (*National Metrology Institute*) for ionizing radiation metrology within EURAMET (*The European Association of National Metrology Institutes*) and it has a long tradition in metrology R&D activities. To mark the start point of its research activity, in this actual form, "MetroMC" conducted a simple theoretical experiment in order to compare the results obtained by approaching the same problem by various Monte Carlo codes that are currently being applied by the group members (MCNP, GEANT4, and EGSnrs). It was shown in recent papers that some inconsistencies between the results obtained by different codes are not related only to the codes themselves, but also to approaching the same problem by different individuals [14].

A brief explanation about the Monte Carlo technique and the used toolkits is presented in Section 2.

The procedure of the theoretical experiment and the obtained results are presented and discussed in Section 3. Finally, a summary of the present study along with the concluding remarks is provided in Section 4.

2. MONTE CARLO TECHNIQUE

Monte Carlo is a powerful modeling tool, which can be used to simulate statistical processes such as the interaction of nuclear particles with matter [15]. This method estimates the solution of mathematical problems by generating numerous random numbers.

It is particularly competent for complex problems that are hard (or impossible) to be modeled by using deterministic methods.

Monte Carlo is indeed a realistic technique, which – in the case of particle transport – actually follows each of many generated particles from the source to the end of its path (absorption, escape, etc.). Simulating individual particles and recording some aspects of their average behavior, Monte Carlo supplies the specific information requested by the user.

Three computer codes, working based on the Monte Carlo method have been chosen for comparison in this study. Following is a brief explanation of each code.

2.1. MCNP

MCNP is a general-purpose Monte Carlo N-Particle transport code, which is developed and maintained by Los Alamos National Laboratory [16]. This code deals with several transport modes: neutron only, photon only, electron only, combined neutron/photon transport where the photons are produced by neutron interactions, neutron/photon/electron, photon/electron, or electron/photon. The energy range is from 10^{-11} MeV to 20 MeV for neutrons, and from 1 keV to 1000 MeV for photons and electrons.

Some important standard features that make MCNP adaptable and easy to use are as follows: Capability to define a wide variety of general, surface, and criticality sources; the ability to plot both geometry and output tally; having an extensive collection of variance-reduction techniques, tally types, and cross-section data.

The geometrical cells in MCNP are bounded by first- and second-degree surfaces and fourth-degree elliptical tori, and can be made from arbitrary materials.

Continuous-energy nuclear and atomic data libraries are included in MCNP. For neutrons, the code takes into account all the reactions given in a particular cross-section evaluation (*e.g.*, ENDF/B-VI). For photons, incoherent and coherent scattering, fluorescent emission after photo-electric absorption, pair production with local emission of annihilation radiation and bremsstrahlung are considered. For electron transport, the code uses a continuous slowing down model that includes positrons, K x-rays, and bremsstrahlung. MCNP uses nuclear data for neutrons and atomic data for photons and electrons.

The version 4C of the code (MCNP4C) has been used in this work, which is applicable in both Unix and Windows operating systems [17, 18].

2.2. GEANT4

Geant4 (GEometry ANd Tracking) is a Monte Carlo simulation toolkit that includes a wide variety of applications in nuclear and particle physics, accelerator design, space engineering, and medical physics. Its high-level functionality allows the user to model the interaction of particles with matter over a wide energy range from 250 eV to 1 TeV with exceptional accuracy. Object-oriented programming is used to achieve clarity and advanced software-engineering techniques in C++ can create a diverse environment.

The most important aspects of the simulation process in Geant4 are: The geometry of the system, the particles and materials of interest, the generation of primary and secondary events, the tracking of particles through materials, the physics processes governing various interactions, the generation of necessary data for the possible events, the storage of events and tracks, the visualization of the geometry and particle trajectories, and the analysis of the output data at different levels of details.

Users can construct stand-alone applications or use other object-oriented frameworks to interact with the environment. Another useful particularity of the toolkit is its capability to support many data analysis programs like Root, gnuplot, Valgrind, etc. To this end, Geant4 includes user interfaces, built-in routines, and command interpreters that operate at each level of the simulation. Due to its many features, Geant4 is a very useful simulation code in metrology, where the need for precise results is inevitable [19]. For metrology applications, in Geant4 (as in other Monte Carlo simulation codes), it is important to use the most reliable and precise nuclear data available [20].

2.3. EGSnrs

EGSnrc is applied to perform Monte Carlo simulations describing the transport of ionizing radiation through matter. The software toolkit comes with a set of packages or classes written in C++, as well as a general-purpose geometry library used for modeling complex geometries and particle sources.

The particles that can be modeled with EGSnrc are photons, electrons, and positrons, with an energy range from 1 keV to 10 GeV. Moreover, a set of particle sources and different propagation algorithms are included in the toolkit.

Originally developed at the *Stanford Linear Accelerator Center* (SLAC) in the 1970s, the *Electron Gamma Shower* (EGS) software was improved to become EGSnrc, which integrates important refinements in charged particle transport, the egs++ class library, and better low energy cross-sections.

Writing an application can be done by using any programming language as long as it can interface with the Fortran EGSnrc code-base. Most commonly, users write their applications in C++ and Mortran3, which is the native EGSnrc language. A reason for this might be that EGSnrc is distributed with several applications written in the previously mentioned programming languages that cover a wide range of calculations such as dose calculations in voxelized phantoms and ionization chamber correction factors [21].

3. BENCHMARK, RESULTS AND DISCUSSION

It is known that water phantom is a good approximation of soft tissue in nuclear medicine and radiation protection-related dosimetry [22, 23]. Therefore, in this paper, a water cylinder was chosen to be modeled by using the above-mentioned simulation toolkits. This is an ideal – although simple – virtual experiment to demonstrate the compatibility of different modeling codes. The water cylinder phantom has a 5 cm radius and 10 cm height. A point γ source is positioned along the cylinder axis and at 25 cm distance from the center of it. The modeled radioactive source emits isotropic and monoenergetic photons with 100 keV energy. The secondary electrons are taken into account in the simulation process. The simulation was performed by MCNP4C, GEANT4, and EGSnrs with 10^7 tracked particles which are called events or histories, depending on the used program. Figure 1 shows a 3D view of the simulated geometry and particle tracks by EGSnrs code. The data of interest is the total absorbed dose in the cylinder volume.

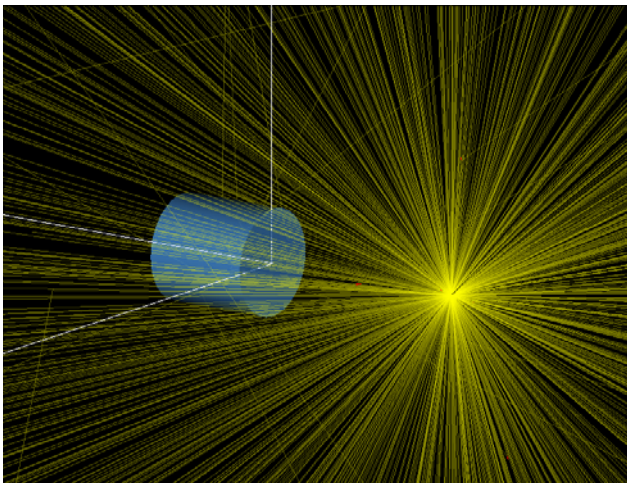

Fig. 1 – Water cylinder, point γ source, and particle tracks (export from EGSnrs).

The obtained results by each Monte Carlo code are given in Table 1. The calculated uncertainty by each code is less than 1%.

The average of computed absorbed dose by simulation codes is calculated and the relative difference between each value and the average (arithmetic mean) is also presented in the table. It can be seen that the bias from the average value in each case is less than 1%, which means the results obtained by using different simulation codes are in a very good agreement.

Table 1

Results of the theoretical experiment, simulated by three modeling codes

Simulation code	**Total absorbed dose ($\times 10^{-10}$) [Gy]**	**Uncertainty [%]**	**Average value ($\times 10^{-10}$) [Gy]**	**Bias [%]**
MCNP4C	4.715	0.43	4.748	– 0.695
GEANT4	4.745	0.33		– 0.063
EGSnrc	4.783	0.43		– 0.737

4. CONCLUSIONS

In this paper, the undisputable needs and the suitability of computational physics in ionizing radiation metrology were highlighted. In order to provide support in this matter, “MetroMC”, a new young research group has been formed. To point out the coherence between the results obtained by the group's members, a benchmark of three different MC codes was performed (MCNP4C, GEANT4, and EGSnrs). In future studies, another toolkit (PENELOPE) will be added to the Monte Carlo-codes group. Having various simulation codes can lead to more reliable results, which is the main goal of the Monte Carlo group. As it was shown, the obtained results (absorbed dose) for the arbitrary chosen model (a 5 cm by 10 cm water dosimetry phantom and a point-like isotropic 100 keV quanta gamma-ray emitting source placed at 25 cm from the center of the cylinder) were in a very good agreement. The relative difference between the individual results (obtained by three different codes) and the mean value (considered as "conventional true value") was under 1%. The statistical uncertainty associated with each individual value was also less than 1% in all three cases for just 10^7 events, which leads MC codes in the "metrological targeted" uncertainty area. This aspect can be even improved by making use of more powerful state-of-the-art computational resources. The MC codes are usually used in metrology in case of complex measuring geometries, restricted availability of some specific radionuclides for different reasons, complex detectors development, uncommon ranges of energy or magnitudes, obtaining correction factors, etc. These codes can be used as stand-alone (after being validated by correlation with experimental data) or complementary to measurements. By correlating the results obtained by models and the experimental data, the traceability (the mandatory metrology condition) is being approached. The importance of using identical input data (same recommended nuclear decay database) as well as good communication between the MC codes users was also pointed out. This aspect can be easier to overcome by working groups as "MetroMC".

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