Applications of the Monte Carlo method in nuclear physics using the GEANT4 toolkit

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Abstract. The capabilities of the personal computers allow the application of Monte Carlo methods to simulate very complex problems that involve the transport of particles through matter. Among the several codes commonly employed in nuclear physics problems, the GEANT4 has received great attention in the last years, mainly due to its flexibility and possibility to be improved by the users. Differently from other Monte Carlo codes, GEANT4 is a toolkit written in object oriented language (C++) that includes the mathematical engine of several physical processes, which are suitable to be employed in the transport of practically all types of particles and heavy ions. GEANT4 has also several tools to define materials, geometry, sources of radiation, beams of particles, electromagnetic fields, and graphical visualization of the experimental setup. After a brief description of the GEANT4 toolkit, this presentation reports investigations carried out by our group that involve simulations in the areas of dosimetry, nuclear instrumentation and medical physics. The physical processes available for photons, electrons, positrons and heavy ions were used in these simulations.

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INTRODUCTION

In the last years numerical simulations have received great importance in almost all scientific areas. Simulations with Monte Carlo methods, in particular, have been employed more frequently mainly due to the availability of high performance computers at low prices. The inherent stochastic behavior of particles and radiation in matter makes the Monte Carlo method a natural tool to simulate their tracks when traversing radiation detectors, shields, and biological tissues. Because of this, several good Monte Carlo codes are presently available to be employed in all nuclear physics problems that involve the transport of particles and radiation.

Among the popular Monte Carlo codes, the GEANT4 [1] is nowadays one of the most complete toolkit, because it includes physical processes to simulate the transport of practically all types of particles. It has been employed in many problems of basic and applied nuclear physics, as instrumentation for low and high energy physics, reactor physics, space science, dosimetry, radiation protection and medical physics.

In the first part of this article some general information about the GEANT4 toolkit

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is presented. Then, some examples of GEANT4 simulations are described, focusing in diverse studies performed by our group. Finally, some remarks and perspectives about the use of Monte Carlo methods in particle transport are conjectured.

THE GEANT4 TOOLKIT

Geant4 is an object-oriented toolkit developed by an international collaboration that can be used to simulate the passage of particles through matter [1, 2]. The code is an open-source distribution available at the web-site `http://geant4.web.cern.ch`. It is written in C++ language and provides a complete set of software components to implement the whole simulation process: geometry description, materials, particles, physical processes, sources of primary particles, generation of event data, and visualization of the geometry and particle trajectories. The toolkit contains a set of physical models to handle the particle interactions with materials. The user must specify, for each particle type, which physical process must be activated in the simulation.

The package includes several examples that can be used as a starting point to build the codes for new applications. A discussion forum is also available, where the users can describe their problems and ask for support. As the code source is free, new functionalities can be implemented by users, according to their necessities, and several of these implementations can be later included in new versions of the source code. In this way, GEANT4 is a package that grows with the users necessities.

EXAMPLES: CASES STUDIED BY OUR GROUP

In this section, studies performed by our group that use simulations are described. Some of these examples present the typical procedures involved in the simulation of an application, which comprise the experiment modeling, the method validation, and the application execution. The experiment modeling involves: the inclusion of the relevant physical parts; the choice of particles, physical processes and parameters; the definition of the primary source; the visualization of the geometry and events. The validation is usually performed by comparing the results with experiments, references, analytical previsions or results of other Monte Carlo codes.

X-ray production

The knowledge of the energy spectra produced by x-ray tubes used in diagnostic medicine is important to optimize the image quality with minimal risk for the patient. The precise measurement of such spectra is a difficult and expensive task, and usually requires laborious procedures. The availability of a confident tool to simulate the energy spectra would be very appropriate and useful. In order to validate the GEANT4 for calculation of energy spectra used in diagnostic medicine, simulations of typical commercial x-ray tubes were performed.

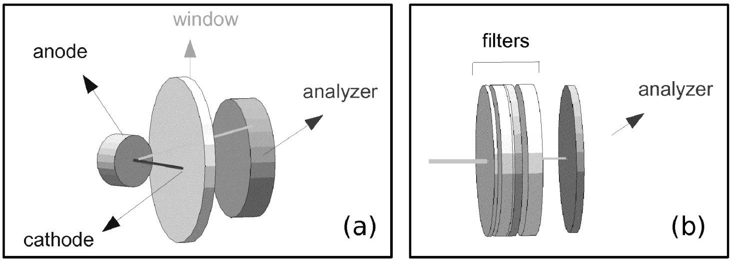

FIGURE 1. Visualization of the simulated x-ray tube (a), and the simulated filters (b) [3].

Figure 1(a) shows the elements of the simulated tube and Fig. 1(b) shows the additional filters [3]. In this simulation the included particles are electrons and gammas. The physical processes employed for electrons are the bremsstrahlung and ionization, while the Rayleigh scattering, Compton scattering and photoelectric effect are used for gammas. Pair production is not activated because the maximum energy is below the threshold. Fluorescence and Auger effect are activated to produce the atomic relaxation after the ionization and photoelectric processes. The primary source is an electron pencil beam with energies corresponding to the applied voltage. Additional filters are used to change the energy spectra of the outgoing photons, depending on the particularities of the diagnostic image.

Figures 2 (a) and (b) show simulated spectra compared with references for high and low filtration, respectively [4]. The simulated spectra shown in the figures were obtained using the physical processes of the GEANT4 Low Energy extension. Good agreement with the reference spectrum is observed in the case of high filtration, where the characteristic x rays of W present weak intensity in comparison with the bremsstrahlung intensity. For the low filtration spectrum the intensity of the characteristic x rays is not

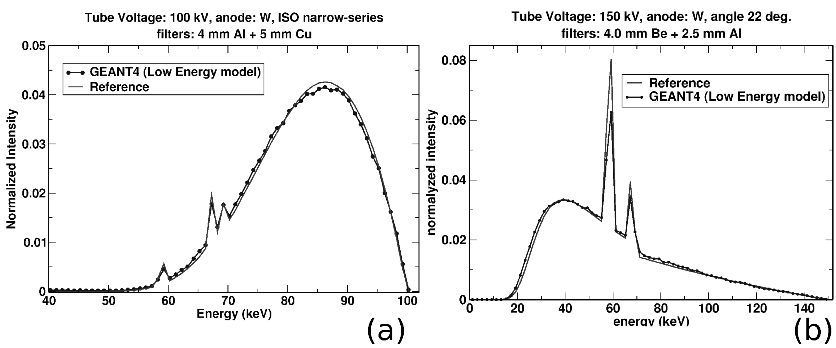

FIGURE 2. (a) Simulated and reference [5] X ray spectra obtained for tube voltage of 100 kV and filters of Al (4 mm) and Cu (5 mm). (b) Simulated and reference [6] X ray spectra obtained for tube voltage of 150 kV and filters of Be (4 mm) and Al (2.5 mm) [4].

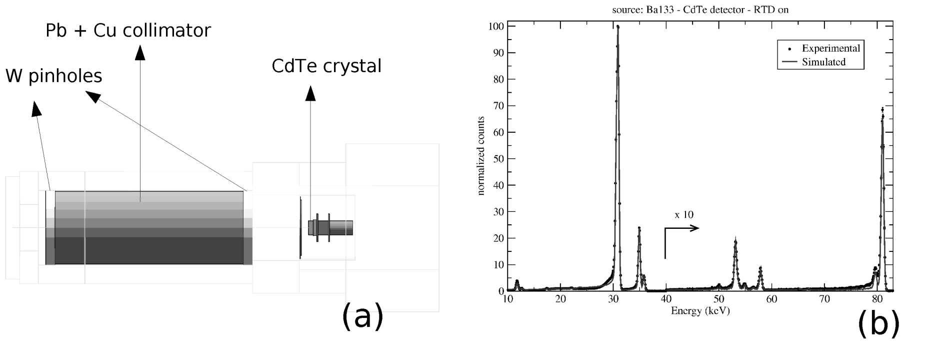

FIGURE 3. Visualization of the complete CdTe detector (a), and the comparison between experimental and simulated spectrum of ^{133}Ba (b).

well predicted by the simulation. This indicates that the balance between the intensities of ionization and bremsstrahlung processes is different for the GEANT4 and Cranley's calculation [6]. Both spectra show the shape of the bremsstrahlung distribution in accordance with the references.

X and γ-ray detection

The simulation of x and γ-ray detection using a CdTe spectrometer was performed with GEANT4. Because of its compactness and good performance at room temperature, CdTe is suitable to be used in field measurements. To calculate the source spectrum of a x-ray tube, unfolding of the measured spectrum must be applied by using a function that describes the detector response, which can be modeled with Monte Carlo simulations [7]. The physical elements of an AMPTEK CdTe detector is shown in Fig. 3(a). Figure 3(b) shows the comparison between the experimental and the simulated spectrum of a ^{133}Ba source. The simulation took into account the bad charge collection presented by the CdTe detector, which was included by using the Hecht equation [7]. One observes good agreement between experiment and GEANT4 simulations.

Medical Physics

Voxelized phantoms can be implemented in GEANT4 applications. In this example, the MAX phantom [8] was included in an application to study the internal dose of activated glass microspheres inserted in the liver of the patient. The microspheres can contain ^{32}P or ^{90}Y radionuclides, which are pure beta emitters.

Using the *GetPosition()* and *GetTotalEnergyDeposit()* methods of GEANT4, the energy deposited in each voxel can be accumulated for all events, and the dose can be calculated for each organ. Table 1 shows the deposited energy and dose for several or-

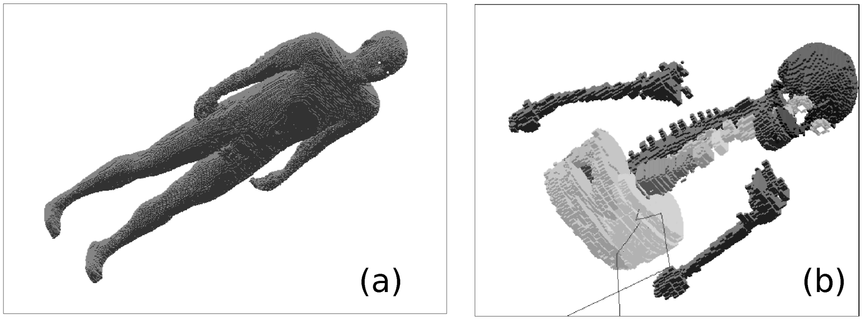

FIGURE 4. Visualization of the complete MAX phantom [8] (a), and the superior part of MAX with some tissues made invisible to show internal organs (b).

gans after the simulation of 1×10^6 electrons of 1 MeV randomly placed in the liver. One can observe that using a pure beta source only the target organ (the liver in this case) receives a high dose compared to other organs.

TABLE 1. Calculation of deposited energy and dose using 1×10^6 electrons of 1 MeV randomly placed in the liver.

Organ	Energy (MeV)	Dose (nGy)
adrenals	5.87	0.067
colon	64.72	0.030
intestine	30.87	0.012
kidneys	41.83	0.023
liver	$\mathbf{9.976 \times 10^5}$	**89**
pancreas	24.50	0.029

Heavy-ion reactions

Another example of application that is in progress concerns the planning of an experiment involving heavy ions. The products of reactions with an ^{4}He gaseous target will be analyzed by silicon $\Delta E - E_{res}$ telescopes placed at forward angles. The aims of the simulations are: to analyze the viability of the experiment, to calculate the energy dispersion of the outgoing particles, to find an optimized target thickness, and to calculate the heat produced in the target. Preliminary studies have been performed using some of the available physics for heavy ions: energy loss by ionization, elastic scattering, inelastic scattering, and fusion-evaporation. To obtain good statistics, a virtual silicon telescope was defined covering the whole forward angle (2π), as shown in Fig. 5(a). Figure 5(b) shows the matrix of the $\Delta E \times E_{res}$ events of a simulation of the ^{8}Be + ^{4}He for E_{lab} = 100 MeV, where the isotopes from H to C can be clearly identified.

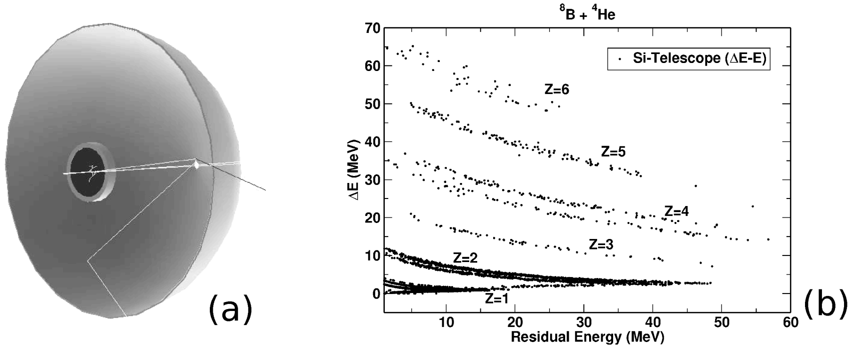

FIGURE 5. Visualization of the simulated telescope (a). The $\Delta E \times E_{res}$ simulated spectrum (b).

FINAL REMARKS AND PERSPECTIVES

The use of Monte Carlo simulations for ionizing particle transport will increase strongly in the next years. Because of the involved social interest, medical applications will give an impulse to the appearance of new codes as well as to the improvements of the existing codes. Monte Carlo simulations will become a common tool in projects of medical instruments (tomography, radiotherapy), planning of radiotherapy treatments (photons, electrons, protons, ions, neutrons) and dose calculation. The needs of more accurate results will require new measurements of cross-sections and the development of better models for the particle interactions. Due to its engineering characteristics and flexibility, GEANT4 will receive many improvements and also new users.

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