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Production threshold impact on a GEANT4 calculation of the power deposition in a fast domain: MEGAPIE spallation target

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Abstract The calculation time in the Monte Carlo simulations consistently represents an essential issue. It is often very long, and its decrease constitutes a challenge for the simulator. Generally, an MC simulation is qualified as quality or not according to two main criteria: the calculation time and the accuracy of the results. However, in most cases, the optimization of one criterion affects negatively the other. Therefore, a compromise between both of them is always required in this kind of simulation. The present work aims at studying the impact of the production threshold (or cut) of the GEANT4 toolkit on the calculation of the power deposition in the MEGAPIE spallation target. The production threshold of secondaries is a GEANT4 intrinsic parameter. It indicates the limit of energy we can reach in the production of secondary particles. This study has allowed us to make the following conclusions. First, the influence of the cut on the calculation of the deposited power depends on the volume size, its arrangement and the importance of the electromagnetic processes occurring within. Second, the accuracy of the calculations can be acceptable only below a given value of the cut energy. Third, this accuracy remains almost unchangeable from a certain value of the cut. The study has also made it possible to explore the prevalence of certain interactions in the zone of spallation in the MEGAPIE target.

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1 Introduction

The Monte Carlo (MC) codes are divided into two classes [1] according to their specific approaches in the particle tracking. Class I gathers the so-called general codes like MCNP [2] that uses the condensed history method [3–6]. Class II gathers codes that mix the condensed method and the detailed one [7]. In the condensed method, the produced interactions and particles in a step are not all explicitly simulated. This method consists of grouping the individual interactions into global steps during which the deposited energy, displacement and direction are sampled from relevant multiple-scattering distributions. Conversely, the detailed method consists of simulating all interactions explicitly so that each step corresponds to one interaction. GEANT4 [8–10], which interests us in this study, is a class II code. In this code, the interactions are divided into two types: hard and soft. The simulation of the hard interactions is performed with the detailed method; whereas, the soft interactions are simulated with the condensed method. The classification of the interactions in class II codes is made according to an energy called "production threshold" [11]. In a GEANT4 simulation, all the particles, primaries and secondaries are tracked down to zero energy. However, the so-called production threshold (cut) limits the generation of the secondary particles. This parameter also acts on the calculation accuracy and on the computing time. The cut is usually taken into account in the low-energy fields, but in this work, we have dealt with this subject in the MEGAPIE spallation target [12, 13]

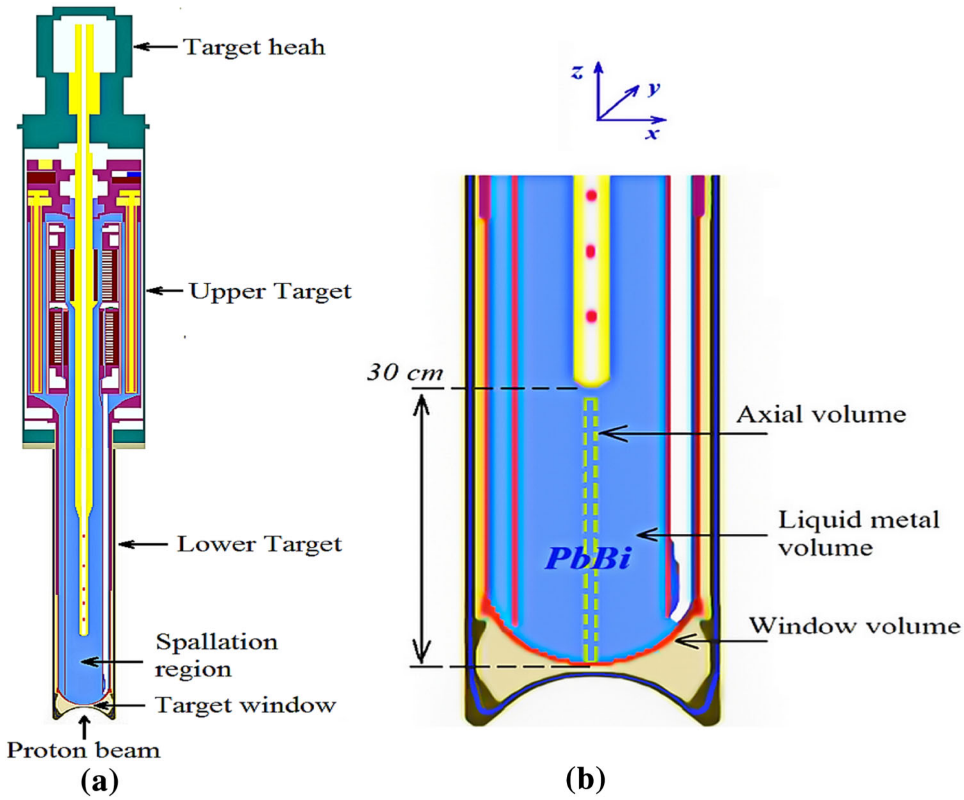


Fig. 1 (Color online) **a** overview of a vertical cut of the geometry of the MEGAPIE target, **b** illustration of the volumes of interest in this study

(Fig. 1a) that is classified as a fast domain 575 MeV. MEGAPIE is an international initiative launched in 1999 in order to design, build, operate and dismantle a high-power (1 MW) liquid lead–bismuth (PbBi) spallation target [13]. Using a GEANT4-based simulation, we have calculated the powers deposited along the z-axis of the target, in its window and in the liquid metal (PbBi) (Fig. 1b). The above powers have a particular interest in the design, the safety and the life of the target. Therefore, it is extremely interesting to evaluate the impact of all the parameters that are able to affect the accuracy of these powers. In fact, the cut is an important one of them.

The selected volumes have different forms, sizes and arrangements. The diversity of these volumes has allowed us to determine the conditions favoring the cut influence on the power calculation.

To evaluate the impact of cut under study, we have compared the results of this simulation with others of reference. The powers taken as references are those calculated and validated in our previous work [14].

2 Materials and methods

2.1 GEANT4 toolkit

GEANT4 (GEometry ANd Tracking 4) is a C++ library designed to simulate the passage of particles in the matter by the MC method. It is a universal code widely used in the world. It covers several physical areas: nuclear physics, particle physics, astrophysics and medical physics. GEANT4 is not a simple code in which the user's role is only to manipulate predefined components, but a very flexible toolkit which is full of features. It offers to the users the possibility to fully customize their own application. Indeed, in a GEANT4 simulation, it is always allowed to make modifications to the available implementations and/or add others according to the problem and equipment needs. On the other hand, the GEANT4 toolkit is used as a basis for some specific codes such as the Gate code [15, 16], the GAMOS framework [17, 18] and the MCADS model [19–22]. Gate and GAMOS are specific for medical applications. Whereas, the MCADS model, developed by FIAS institute in Germany, is intended to simulate the spallation targets.

In the present simulation, we have used the GEANT4 v10.2 [11]. This version has brought several improvements, in particular, the compatibility with parallel calculations. GEANT4 proposes two kinds of parallelism: clustering

[23] and multithreading [24]. Clustering refers to the parallelism with separate memory that requires multiprocessor equipment, while multithreading is a parallelism with shared memory that requires multicore processors. In this work, we have adopted the multithreading technique, which is based on the optimization approach of the memory management. Using this technique, it has been possible to reduce the computing time by a factor that is almost equal to the number of cores. To ensure an optimal functioning of the GEANT4 toolkit, we have built the GEANT4 v10.2 version in an environment constituted by: The scientific Linux v7.4 [25], the class library for high-energy physics CLHEP v2.3.1.1 [26], the data analysis framework ROOT v6.12 [27] and the development framework Qt v5.6.2 [28].

Our simulation is performed using an application with many input files. In these files, the physics, geometry, materials, source (proton beam) and the result extraction methods are all described explicitly with the C++ language or by using command lines. The physics models, the geometry of the MEGAPIE target and the distribution of the proton beam used in this work are the same of those given in our publications [29].

2.2 Production threshold (cut)

As it has been mentioned above, there is no tracking cut energy "cutoff" in GEANT4. All the particles are tracked down to zero energy. However, there is another concept adopted by GEANT4; it is the cut. This threshold is the energy below which it is not allowed to produce some secondary particles. Indeed, when the projectile particle has an energy lower than the threshold, the interaction which gives rise to a secondary particle is considered a continuous loss of energy. The secondary particles concerned by the cut are electrons, positrons, protons and gamma rays (e^-, e^+, p, and γ). The threshold energy depends on the type of the particle and the crossed material. To avoid this dependence, the cut is given as a distance called the "range-cut." Any particle that is unable to travel at least this distance (range-cut) is not generated. In a GEANT4 simulation, it is possible to define only one range-cut for all the particles (e^-, e^+, p and γ) or specify one for each type of particles and/or each region of the simulated geometry. The defined range-cut is transformed into energy thresholds by the code at the beginning of the user code execution [11, 30]. In the user code, the definition of the range-cut can be performed either in the **SetCuts()** or as command lines in a macro-file. The **SetCuts()** method is implemented in the user physics list class which is derived from **G4VUserPhysicsList** class.

The cut is a GEANT4 parameter which acts on the accuracy of the simulation, the calculation time and possibly on the convergence of certain physical processes. The magnitudes whose accuracy is affected by this parameter are, in particular, the power deposition, the electron spectrum and the photon spectrum. The more the threshold value decreases, the more the number of simulated particles increases. Generally, when the number of simulated particles increases, the results become more accurate, but at the same time, the computing time becomes increasingly long. Nevertheless, if the cut reaches very low levels, ultra-soft photons are generated. This generation leads to a divergence in the determination of the final state. Such phenomenon is called "infrared divergence." The different effects of the cut are studied a lot in low-energy GEANT4 simulations [31–34]. Nevertheless, the subject is rarely approached in high-energy domains although it appears interesting as it is shown in this study.

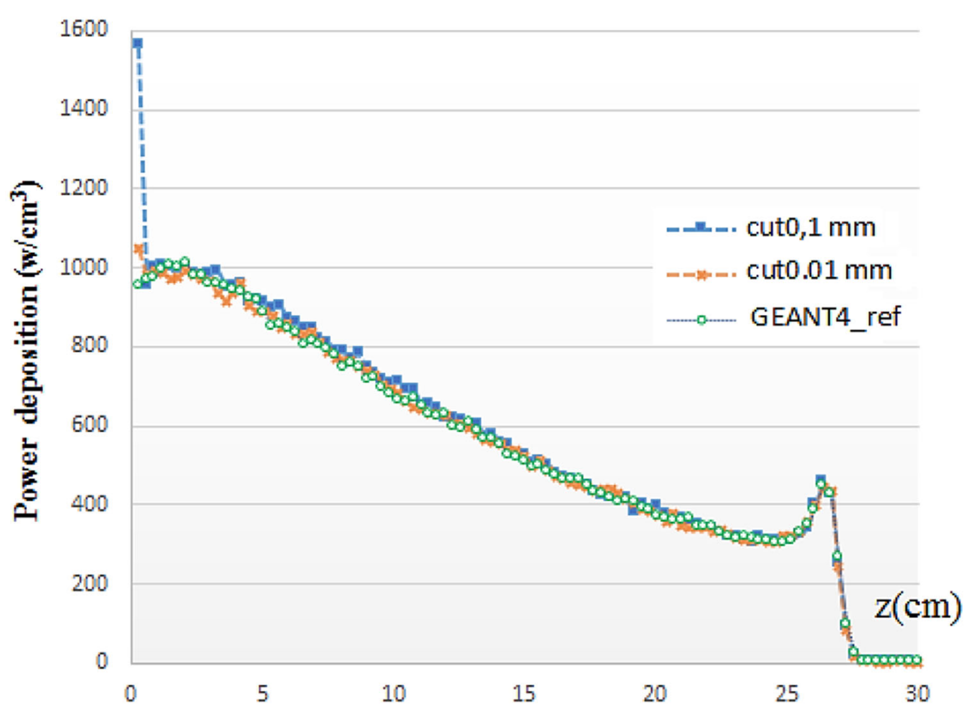
In this work, we have tested a set of cuts ranging from 0.1 μm to 1 m. The reference results with which the comparison is made are calculated with the following thresholds: 0.5 μm for the axial zone of the target, 0.1 μm for its window and 10 μm for the liquid metal PbBi. The differences between these thresholds are due to the differences in the dimensions and orientations of the concerned volumes.

3 Results and discussion

In addition to the spallation reaction, the passage of the proton beam through the MEGAPIE target induces several other particle–matter interactions. Indeed, after its penetration in the target, the proton undergoes initially electromagnetic interactions and subsequently nuclear interactions. Obviously, the spallation reaction is one of these nuclear interactions. In general, the strong nuclear collisions could be perceptible only after a certain penetration distance. This distance is merely the corresponding mean free path. For the heavy charged particles, like the proton, the mean free path for strong nuclear collisions is generally large [35, 36]. For this reason, the proton beam loses an important part of its power via the electromagnetic processes before it interacts with the nuclei of the medium. The concerned electromagnetic processes are in particular ionization, excitation, Coulomb scattering and the bremsstrahlung. When the proton or any other charged particle dissipates an amount of its energy in the target by such processes, the released secondary particle transports part of this energy to other places of the target. However, in a GEANT4 simulation, the secondary particles (e^-, e^+, p and γ) can achieve this role only if the defined value of the range-cut allows their generation. If the generation is not allowed under the range-cut condition, the energy that the projectile charged particle exchanges with the target is deposited totally in the interaction position. Consequently, the topology of the energy deposition in the target is affected as shown in Figs. 2 and 3. These figures illustrate the distributions of the power deposition along the z-axis of the MEGAPIE target for different range-cuts. Figure 2, where the cut $\leq$ 0.1 mm, shows that the graphs coincide with the reference graph, except the nuance noticed in the first 3 mm. This nuance has almost no impact on the rest of the results. However, the gap with the reference graph becomes increasingly large as the cut increases (Fig. 3). From the cut = 10 mm, the difference reaches its maximum ($\sim$ 40%). Nevertheless, this great difference is only noticed on a distance of approximately 10 (cm) from the target window. The remaining zone of interest from the power deposition point of view: 10 cm $< Z <$ 27 cm, can be divided into three parts: 10–14 cm, 14–25 cm and 25–27 cm. In the part 10–14 cm, the increase in the cut slightly affects the deposited power. However, in the part 14-25 cm, the variation of the cut does not have practically any effect on the calculation of the power deposition. In the last part 25–27 cm, the impact of the cut reappears again in a way that the induced difference reaches 14% without moving the Bragg peak. Finally, it is necessary to indicate the presence of large peaks in the graphs corresponding to cuts $\geq$ 1 mm. These peaks are very salient and are repeated in an almost periodic way in the zone 0–14 cm (Fig. 3).

The analysis of the curves made above can be interpreted as follows: The important fall of the deposited power in the zone 0-10 cm means that the secondary particles strongly contribute in the distribution of the power deposition. These secondary particles are not generated because of the elevation of the cut. The extremely large peak at the beginning of this zone indicates that the concerned secondary particles are mainly born at the entrance of the target. In other words, the first physical processes, undergone by the protons in the target (PbBi), are electromagnetic ones. However, the fact of prohibiting the creation of the secondary particles (e^-, e^+, p and γ) makes all the involved energy deposit close the target window and consequently gives the first peak. The pseudo-periodicity of the peaks in case cut $\geq$ 1 mm (Fig. 4) shows that there is a regeneration of the phenomenon observed at the entrance of the target. This means that new generations of particles with similar characteristics to those of the primary proton beam are produced just before the peaks. Since the spallation reaction is the only candidate able to give rise to this kind of particle generation, then the positions of the peaks also represent the focus of spallation. Obviously, the first peaks and the Bragg one are not included. The decrease in the peaks maxima is explained by the fact that the produced particles in each new spallation are generally slower. These particles are, of course, responsible for the next spallation. It is also remarkable that the peaks preceded by a spallation reaction are followed by an increase in the deposited power. This increase is due to the increase in the fluence of the hadrons, which are in turn due to the spallation reaction [35]. Beyond $Z = 14$ cm, there are no more peaks like the precedents, so there is no more spallation, or at least its impact becomes negligible. The lack of spallation after $Z = 14$ cm is due to the fact that the

Fig. 2 (Color online) Distributions of the power deposited in the z-axis volume of the target for reference cut, 0.01 mm and 0.1 mm



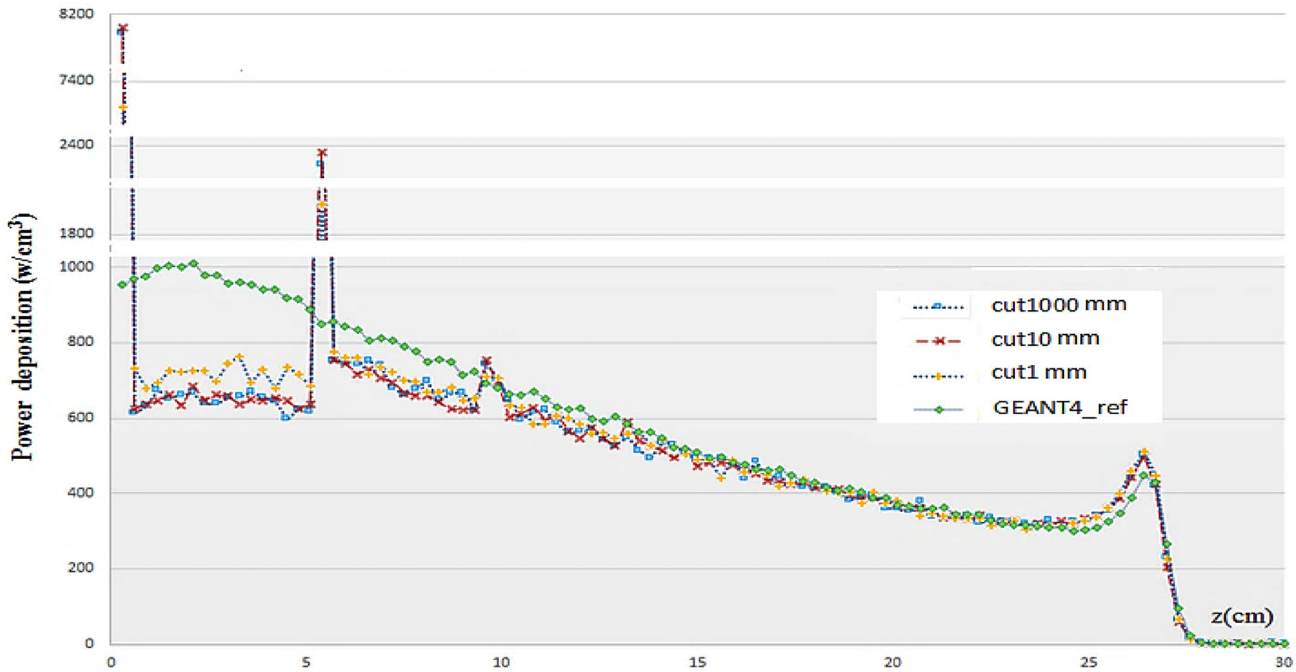


Fig. 3 (Color online) Distributions of the power deposited in the z-axis volume of the target for reference cut, 1 mm, 10 mm and 1000 mm

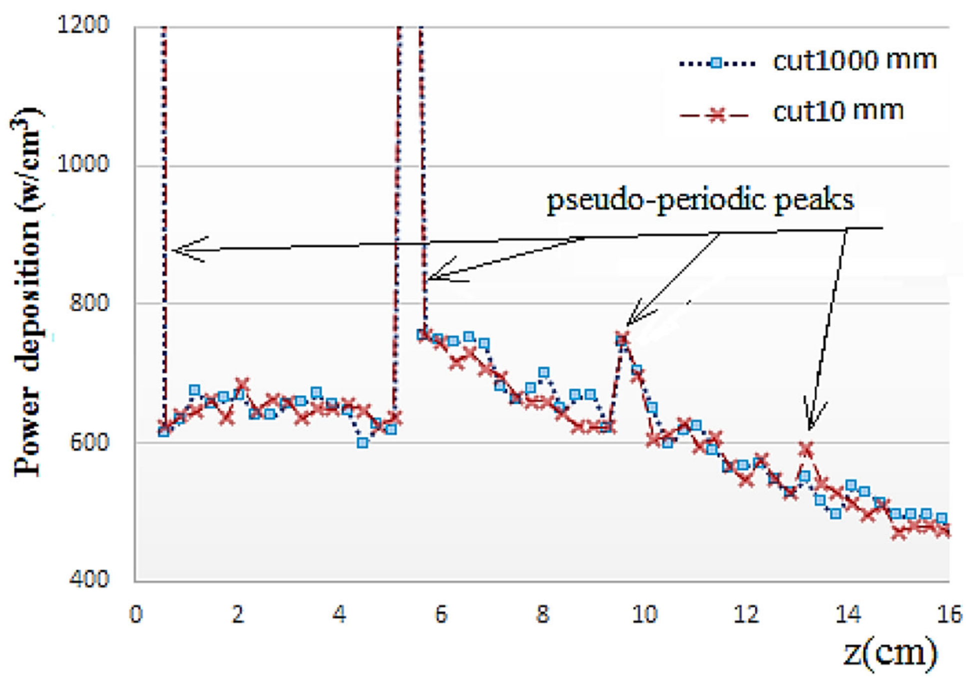


Fig. 4 (Color online) Illustration of the pseudo-periodicity of the peaks in graphs corresponding to high cuts 10 mm and 1000 mm

particles which induce it do not have yet the kinetic energies that promote this type of reaction. Thanks to the multiple spallation produced before, the neutrons become more abundant after Z = 14 cm. Consequently, the neutronic processes become dominating, namely fission, multiplicity, elastic and inelastic scatterings. The predominance of these processes is also justified by the absence of the impact of the cut in the zone 14 cm < Z < 25 cm. Actually, the cut has an effect only when electromagnetic processes occur in a considerable way, which becomes remarkably close to the Bragg peak 25 cm < Z < 27 cm. In this zone, all the particles approach their stops. Figure 3 shows that the secondary particles, particularly electrons and photons, produced in this part do not exceed a range of few millimeters.

The impact observed for the axial volume of the target and discussed above is not the same for all volumes. Indeed, when the volume is broad or arranged crosswise in comparison with the direction of the primary beam, the impact of the cut becomes negligible. Although the spatial distribution of the power deposition in large volumes depends strongly on the choice of the cut, the total power deposited remains almost the same. For instance, the maximum error induced by the variation of the cut in the liquid metal (PbBi) volume, which is large, is less than 0.2% (Table 1). Regarding the thin transverse volumes, particles cross so quickly that it is difficult to induce sufficient electromagnetic processes to influence the power deposition. Figure 5 illustrates the distributions of the power deposition in the target window, which represents an example of these volumes.

On another side, the GEANT4 simulations are, in general, slow and take too much time to be run. Usually, one resorts to the parallelism techniques to reduce the computing time. However, the ability of the users' equipment is often limited although the parallelism techniques allow a strong decrease in the calculation time. Then, the remaining solution to optimize the computing time is to refine the user code and to improve the simulation parameters. In our case, the reduction in this time is based on the multi-threading parallelism technique and on the optimization of the cut parameter. Table 2 summarizes the consumed times in the faster simulation (cut = 1000 mm) and in the reference one.

Table 2 shows that the influence of the cut on the computing time is quite important in the axial volume ($\sim$ 9%) and is more or less significant ($\sim$ 3%) in the PbBi volume, but it is negligible (< 1%) in the window volume. The very low effect of the cut on the computing time in the target window is caused by the fact that this volume is narrow and the power deposition within is almost independent from the cut. The non-negligible saved time (3%) in the case of the PbBi volume is due to the large size of this volume. Finally, the important saved time (9%) in the axial volume is justified by the strong impact of the cut on the power deposition in this volume (Fig. 3). However, this later gain of time is accompanied by a total loss of the calculation accuracy in some areas. That is why one can benefit from the above reduction in the calculation time in the areas where accuracy is not or slightly affected, as in 10 cm $< Z <$ 25 cm.

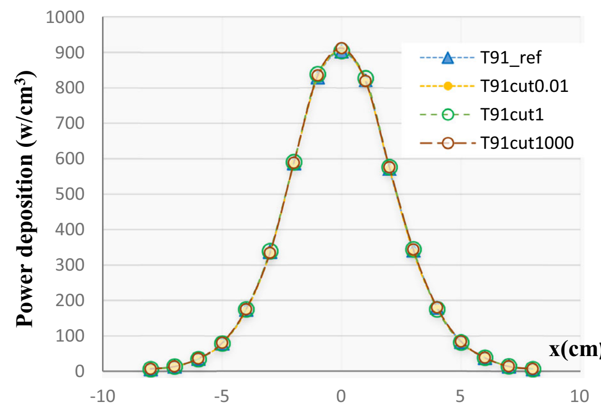


Fig. 5 (Color online) Distributions of the power deposited in the window volume of the target for reference cut, 0.01 mm, 1 mm and 1000 mm

4 Conclusion

In this paper, we have approached the impact of the cut in a GEANT4 simulation aiming at the calculation of the power deposition in the MEGAPIE spallation target. This kind of study is very widespread in the low-energy fields, namely the medical field, but it is very rare in the high-energy fields like the MEGAPIE spallation target. This study has led us to conclude that even in this fast field the cut can play a decisive role in terms of accuracy (Figs. 2 and 3) and reduction in calculation time. The powers evaluated above show that the effect of the cut requires three conditions: The volume in concern must be narrow and oriented according to the primary beam direction. The electromagnetic processes induced in this volume must be able to contribute considerably in the transfer of power. To increase the cut is automatically to eliminate the production of certain particles. These would have been responsible for transporting an amount of energy to other places of the medium. Then, when the considered volume is narrow, this energy will be counted wrongly deposited by the primary particle inside or outside this volume. The fact that a volume has a similar direction with the primary beam gives more chance to particles to be inside this volume longer or several times. Consequently, the probability to induce electromagnetic interactions in this volume becomes higher. Nevertheless, the size of the volume and its orientation by themselves are insufficient to insure the impact of the cut on the power deposition. It is necessary that the type of the particles and their energies correspond to

Table 1 Deposited power in the liquid metal PbBi for cuts 0.01–1000 mm

Cuts (mm)	Ref_Value	0.1	1	10	100	1000
Deposited power in PbBi (w/cm^3)	709.7	709.6	710.2	710.4	710.6	711.0

Table 2 Summary of the consumed times in the faster case and in the reference one

	Volume	Number of events in (1.e+6)	Computing time in (h)		Saved time in (%)
			Reference case	Faster case	
Run 1	Axial	6	135.8	123.67	8.93
Run 2	Window	15	340	336.67	0.98
Run 3	PbBi	6	138.8	134.7	2.95

important cross sections for electromagnetic processes in the crossed medium.

The present study also made it possible to explore the areas of prevalence of certain types of interactions along the axis of the MEGAPIE target. Indeed, the ionization prevails at the beginning of each contact of heavy charged particles with the target. That is distinctly visible in the positions of peaks (Fig. 3), where the charged particles are rather numerous and fast, namely the entrance of the target and the spots where the spallation reactions occur. At the entrance, the proton beam has just arrived at the target. In the spallation reaction spots, new generations of fast particles are born: in the intra-nuclear cascade phase. Since the positions of the peaks, except the first and the Bragg ones, are also the more probable positions for spallation, the spallation zone in the MEGAPIE target is mainly bound by 5 cm and 15 cm. In the exit of this zone of spallation, neutrons become much more numerous and faster than other particles notably protons, so neutronic processes predominate.

Regarding the calculation time, it has been found that the cut can have a considerable influence only if it has an impact on the power deposition or if the concerned volume has a large size. However, the influence is more important in case the cut affects the power deposition as in the axial volume. Finally, we can conclude that the cut, as a GEANT4 parameter, plays an important role in the calculation of the power deposition and in the reduction in the computing time. Moreover, it is possible to explore the predominance of some interactions in the simulated volume using this parameter.

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