GEANT4 Modeling of the International MEGAPIE Experiment

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Abstract

The accelerator driven system (ADS), is an innovative subcritical reactor dedicated to the incineration and the transmutation of nuclear waste. The operation of this reactor is based on an external neutron source, which is a spallation target. In this paper, we modeled the international MEGAPIE (MEGAwatt PIlot Experiment) spallation target by the modern code: GEANT4, work that has never been done with this code. The simulation is performed using several techniques to describe, first the very complex geometry of the device and second the distribution of the proton beam feeding the target. About physics, we used the most suitable physics list for the problem. Concerning the data analysis and the user interface, we exploited the toolkit Qt and the library ROOT. The simulated geometry and proton beam are in good agreement with the real geometry and with the reference beam. To validate the simulation we calculated the power deposited along the z-axis of the target, which leads to excellent results compared to benchmark results. Finally, this work represents a very hard and essential stage towards a total neutronic study of the MEGAPIE target and its optimization with the powerful code GEANT4.

Keywords: GEANT4, MEGAPIE, spallation target, power deposition, modeling

1. Introduction

The toolkit GEANT4 is a modern code, benefits of the new technology of object-
oriented programming. GEANT4 is developed in the framework to respond to the increasing demands of physical experiments, in terms of complexity and sensitivity of the detectors and consequently the power of calculations. GEANT4 is a powerful code, but it is very difficult and requires thorough knowledge of C++ object oriented programming. In this paper, we have taken advantage of the possibilities offered by GEANT4, to model the MEGAPIE spallation target of SINQ installation in Switzerland. MEGAPIE is a liquid metal target PbBi that has a high complex geometry (figure 1). This target is yet in phase of development and testing to build a neutron source, for feeding the future accelerator driven systems (ADS). These reactors are designed to incineration and transmutation of radioactive waste. The materials and the methods adopted in this work, are explained in the section, "Materials and Methods", while the section, "Results and Discussion", is reserved to illustrate and discuss the results. The performed modeling has led to satisfactory results, for the target geometry, the profile of proton beam and the power deposition.

2. Materials and Methods

– GEANT4

GEANT4 (GEometry ANd Tracking 4), is an open source library, coded in C++, containing a very wide range of physical models, physical processes, geometries capability, materials, databases... This diversity offers users the possibility to choose the suitable tools, to achieve their simulations by the Monte Carlo method, each according to the needs of its application area. GEANT4 was designed initially for the experiences of high-energy physics, but it is quickly expanded to cover several areas of physics. It is currently applicable in the particle physics, nuclear physics, astrophysics, medical physics and even for the calculations of the deposition energy at the nanoscale: GEANT4-DNA project. GEANT4 is actually the result of an international collaboration, bringing together physicists and computer scientists, divided into seventeen working groups. These latter ensure the development of the code, the maintenance, the documentation and the assistance for the users of the code, via online forums [1]. More details can be found in [2, 3].

Figure 1: Overview of the MEGAPIE target modeled by GEANT4
Physics list
As GEANT4 covers a broad range of applications, it does not provide physical models by default, but it is up to the user to choose, what model to use and for what process [8]. For modeling the transport of particles in the energy range of the MEGAPIE target, we have chosen the predefined physics list FTFP_INCL++_HP, including the model Intra-Nucleare Cascade of Liege (INCL), and the model High Precision (HP) for modeling processes of interactions of neutrons low energies. However, the model INCL does not manage quite well the energies lower than 150MeV that is why it is coupled with the model ABLA. The choice of this list of physical is justified by the fact that the coupling INCL/ABLA is currently considered the best model for the spallation reaction. It is validated by comparison with the experimental data for several heavy elements [9] and the validation results are in the benchmarks of the IAEA [10].

Geometry of the device (MEGAPIE target)
One of the main objectives of this work is to describe, as realistic as possible, the geometry of the MEGAPIE spallation target figure 1. The definition of the geometry in GEANT4 must be carried out in three steps: Description of the geometric shape, designated by the name solid volume. Assignment of the material composition to this volume, it is the logical volume. The positioning of this latter represents a third concept: it is the physical volume. The richness of the GEANT4 library by predefined geometric shapes and by associated features, has allowed us to reproduce the complex geometry of the MEGAPIE target. This target is built with a large number of geometric elements that have different shapes. The implementation of the geometry is done by using the basic shapes (cylinder, sphere, parallelepiped…), the complex shapes (truncated cylinder, polycone, toric shape, trapezoid…) and the Boolean shapes (obtained by Boolean operations). GEANT4 offers the latter potential feature via three dedicated classes: G4UnionSolid, G4SubtractionSolid and G4IntersectionSolid. The Boolean operations are applicable; either on two simple forms or on forms obtained themselves by these operations.

Definition of the source (proton beam)
To define the source in a GEANT4 simulation, one can use the G4ParticleGun class or G4GeneralParticleSource class. The first class is suitable for several applications; however, a more sophisticated definition requires the use of the second one. In this work, we have chosen the G4GeneralParticleSource class. It allows to specify spectral, spatial and angular distributions of the primary particles source [8]. The MEGAPIE target is powered by a mono-energetic protons beam of 575MeV. Its distribution is plane closely double Gaussian. Several studies have been done using approximate formulas to describe the profile of the proton beam. The following formula is already used by the scientific community hosting the MEGAPIE project (Paul Scherrer Institute in Switzerland).
\[ I_{xy} \left[ \mu A \text{cm}^{-2} \right] = \frac{I_0}{2\pi \sigma_x \sigma_y \left( 1 - e^{-\frac{c^2}{\sigma_x^2}} \right)} e^{-\frac{1}{2} \left[ \left( \frac{x}{\sigma_x} \right)^2 + \left( \frac{y}{\sigma_y} \right)^2 \right]} \]  

Where \( \sigma_x = 3.3 \text{cm} \), \( \sigma_y = 1.9 \text{cm} \). The beam is truncated at \( c \times \sigma_x \) \( (c=2) \). For \( I_0 = 1.74 \text{mA} \).

In this work, we defined the beam distribution by superposition of a large number of plan distributions. The implementation is made via the G4GeneralParticleSource class through a set of commands line included in a macro file.

3. Results and Discussion

- Geometry

The MEGAPIE target is a device that has high complex geometry. It is constituted by many elements and many geometric forms. The upper part of the target is dedicated to the heat removal, so it has mainly a thermal hydraulic interest. Nevertheless, quite a few nuclear phenomena occur there, such as neutronic activation, radioactive decay and especially \( \gamma \) radiation. The more important elements in this part are the upper target enclosure (with stainless steel: SS316L), the electromagnetic pumps, the upper liquid metal container (ULMC), the heater exchanger, the expansion tank, the oil and heavy water boxes, the shielding parts and the target head (figure 2).

![Figure 2](image-url)

**Figure 2:** Some interesting elements in the upper part of the target. (a) Electromagnetic pumps; (b) Upper liquid metal container and heat exchangers; (c) Oil, heavy water distribution boxes and densimet shielding
The lower part has mainly a neutronic interest, because that is where the spallation reaction occurs. The principal elements constituting the lower part are the guide tube (AlMg₃) for the proton beam with 4mm thickness, lower target enclosure (LTE) with double walls of 3mm thickness each (AlMg₃). The two walls are separated by 4mm of heavy water D₂O. The enclosure consists of a cylindrical part and a convex spherical part at the bottom. An isolation volume (IG) of 6mm thickness has the same form as the enclosure, filled by helium gas at 0.5bar pressure in mean. This volume separates the enclosure and the lower metal container (LMC), which also consists, of a cylindrical part with 2mm/4mm thickness (respectively in the spallation region and in the rest) and a concave spherical part. This latest represents the entry window of the proton beam to the target. Inside the LMC, there are the main flow guide tube and the by-pass tube as well as the tubes of filling and drainage, plus the central rod (figure 3). To avoid leakage of neutrons, the spallation region is surrounded by the heavy water, as moderator and the light water as reflector (figure 1). More details about the geometry design of le MEGAPIE target can be found in [4].

The definition of the geometry was a hard task. Firstly, because it requires a very long program (several thousands of lines) and secondly because it requires great care, especially in the positioning of the large number of volumes and in their overlaps. In addition, many volumes have non-simple form, such electromagnetic pumps, connecter flanges, oil boxes, drainage tube and the by-pass duct that have toric forms and the guide tube with slanted section …. These volumes are mainly modeled using Boolean operations (union, intersection and subtraction). To use these operations, it necessary that the argument solids have a good intersection between them and should not overlap or share surfaces with their mothers' volume. Ultimately, the modeled geometry reflects largely the actual geometry of the MEGAPIE target as shown in the figures above.

− Definition of the source (proton beam)
Precise results for Monte Carlo computations of different magnitudes (neutrons spectrum, power deposition …) require a good knowledge of the proton beam profile [11]. To this aim, two approaches are used, one determine the profile by
calculations and one by measurement. About measurements, they were carried out, after irradiation and extraction of the target, by $\gamma$ mapping technique [5]. As mentioned above (cf.:2), we described the source of protons by Monte Carlo method as a set of superposed sources. Each source has its own shape and intensity. The physics magnitudes calculated by modeling are very sensitive to le beam distribution. That is why any error in the choice of these parameters (shape and intensity) makes the calculations wrong. Judicious choices allowed us to describe the spatial distribution of the proton beam, where the illustration are given by the figures (4, 5). A comparison of these results with those of reference,

![Figure 4](image1.png)

**Figure 4:** illustration of the two and three-dimensional proton beam

![Figure 5](image2.png)

**Figure 5:** Profiles of relative current intensity as a function of $(x,y=0)$ and $(x=0,y)$

given in [11] shows, in general, a good agreement. In addition, the accurate results obtained by the present simulation, as shown on the calculation of the power deposition below, confirm this conclusion.
– **Power deposition**

The validity of the program requires that the calculations lead to correct results. To this end, we evaluated the power deposition, along the z-axis of the target. This quantity is one of the most critical magnitudes in the target design. Indeed, the stress of the target material is mainly related to the amount of energy deposited in. The calculation of the power deposition depends, of course, on the description of the geometry and source of protons and in addition, on several physical parameters, especially the cut-off energy. This later parameter is an energy threshold of secondary particles production. It has a strong on the determination of the power deposition, especially in the narrow volumes, as in our case where the volume is a cylinder with 2mm of diameter. The threshold which allowed us to have a good result is 1μm. The power in question is already calculated for MEGAPIE target and validated by several other codes except Geant4 such as FLUKA and MCNPX… The Figure 6 shows a comparison between our results and those calculated by reference codes FLUKA and CFD [6] (these are a benchmark results). It is found

![Figure 6: Power deposition along the z-axis, calculated by FLUKA, CFD(CFX-4.3) and by GEANT4.](image)

that the agreement is excellent between the different results and the relative error is less than 1%. We can also make more comparisons with other benchmark results given in [12]. Anyway, there is a satisfactory agreement with all. Thing that confirms the accuracy of the modeling work, i.e. the accuracy of the geometry, the distribution of de proton beam (source) and of course, the judicious choice of physics lists.

4. **Conclusion**

The significant results obtained in this work whether at the level of the geometry, the source or the power deposition reveal the quality of the modeling work full of planning, programming and structuring. Although the GEANT4 code is highly flexible, rich in features and covers a wide range of energy, it remains one of the
most difficult codes to manipulate. In addition, The GEANT4 requires an advanced knowledge of C ++ object-oriented programming and it is up to the user to write completely his own program with this language. At the end, this work which has never been done by GEANT4, constitutes an essential and laborious task to any neutronic study of the MEGAPIE spallation target. It is the first step towards an optimization of the MEGAPIE target with the powerful an modern code GEANT4.

References


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