PUFI: A TOOL TO PREPARE GEOMETRY FILES FOR PENELOPE MONTE CARLO SIMULATION IN GAMMA-RAY SPECTROMERY

Abdellah Wadjinny, Marie-Christine Lépy*

CEA, LIST, Laboratoire National Henri Becquerel (LNE-LNHB), Bât. 602 PC 111, CEA-Saclay 91191 Gif-sur-Yvette Cedex, France

Keywords: Monte Carlo simulation, PENELOPE, gamma-ray spectrometry

Abstract

The practical use of the general-purpose Monte Carlo code PENELOPE requires the careful preparation of input geometry files to define the experimental conditions. The structure of the geometry file is strictly formatted and the correctness of the geometry definition can be difficult to achieve for new users. Thus a practical interface PUFI (PENELOPE User-Friendly Interface) has been designed to facilitate the preparation of the geometry files for typical cases of gamma-spectrometry simulations with a cylindrical symmetry including detector, volume source and shielding.

1. Introduction

PENELOPE (Salvat, 2015, Salvat and Fernández-Varea, 2009), is a general-purpose Monte Carlo code which allows simulation of coupled electron-photon transport: it is widely distributed for a wide range of applications in the energy range from a few hundred eV to about 1 GeV. Among these, it is of interest to derive practical information in gamma-ray spectrometry, such as optimization of geometrical arrangement, calculation of detection efficiency, self-attenuation transfer factors or coincidence summing corrections.

PENELOPE must be launched with a steering program, which controls the geometry and the tracking of particles, keeps score of all relevant information, and performs the required averages at the end of the simulation. Two typical steering programs are provided in the distribution package of PENELOPE: PENCYL (which simulates electron-photon transport in cylindrical geometries) and PENMAIN (for generic quadric geometries). In each case, the practical use of PENELOPE requires the careful preparation of input geometry files to define the experimental conditions, generally including different sources and detection and/or absorbing materials. The PENCYL geometry structure is quite simple and easy to implement and its use is recommended for simple cylindrical geometries, since only one input file (including both geometrical and simulation conditions) is necessary. However, to cope with more general cases, the user must use PENMAIN, which requires two input files (one for the geometry, and one for the simulation conditions). In this general case, the structure of the geometry file is very strictly formatted, using quadric surfaces which define different interaction bodies, and the geometry can be difficult to correctly define for new users.

Thus a practical interface PUFI (PENELOPE User-Friendly Interface) has been designed to facilitate the preparation of the PENMAIN geometry files for typical cases with a cylindrical symmetry which include the detector, a volume source and different absorbing materials and shielding. The detector is cylindrical (or a rounded-shape) and can include an internal hole; the volume source can be cylindrical or a Marinelli-type, and the external shielding is cylindrical.

2. PENELOPE input files

The geometry is defined from a text file, which consists of a sequence of blocks defining the different elements (surfaces, bodies or modules) according to a specific format. First, limiting surfaces must be defined: in the case of a cylindrical geometry, these are either planes or cylinders, as shown in Figure 1.

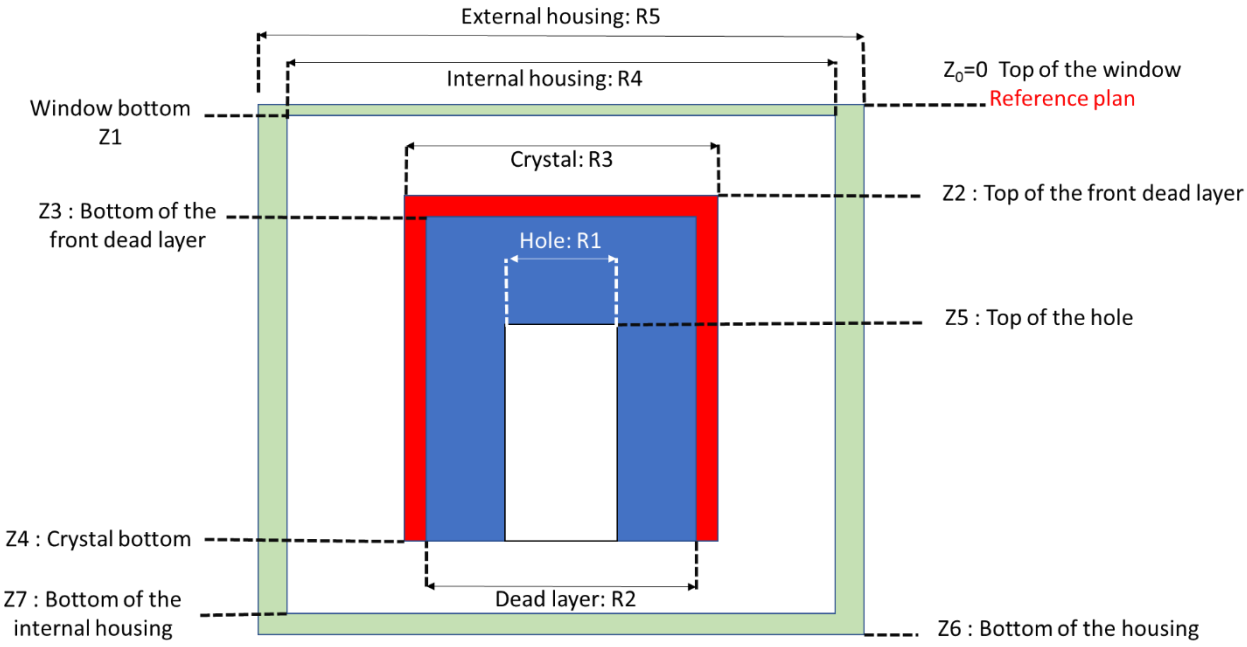

Figure 1: Typical limiting surfaces in the case of a cylindrical detector

The different "bodies" are then described from the intersection of the pre-defined surfaces. It is necessary to start from the internal bodies and to add successive elements, thus the detector and the source must be defined before including these in the shielding. However, the geometry input can be tedious and errors may be caused if the format strict structure is not followed.

3. PENELOPE User-Friendly Interface (PUFI)

PUFI is an acronym for PENELOPE User-Friendly Interface which was prepared using the Python language. It has been conceived to prepare PENELOPE geometry files in an easy way. As already mentioned, the file structure is specifically formatted and the construction of the geometry must follow an order to mention if there are some intersection between the different bodies. With PUFI, only the typical dimensions of the experimental elements and their relative position are required, and must be input according to a specific order, from internal elements (detector) to external ones (shielding). It should be noted that all dimensions must be entered in millimeters by the user; they are automatically converted into centimeters to cope with the

PENELOPE requested format. The PENELOPE geometry file is automatically generated from these elements and the resulting geometry can be verified using the PENELOPE visualization tool (PenGeomjar (Almansa *et al*., 2016)).

4. PUFI practical use

As for any geometry definition, it is recommended to prepare a draft scheme of the experimental arrangement to determine the different elements, materials and relative positions, as presented in Figure 2:

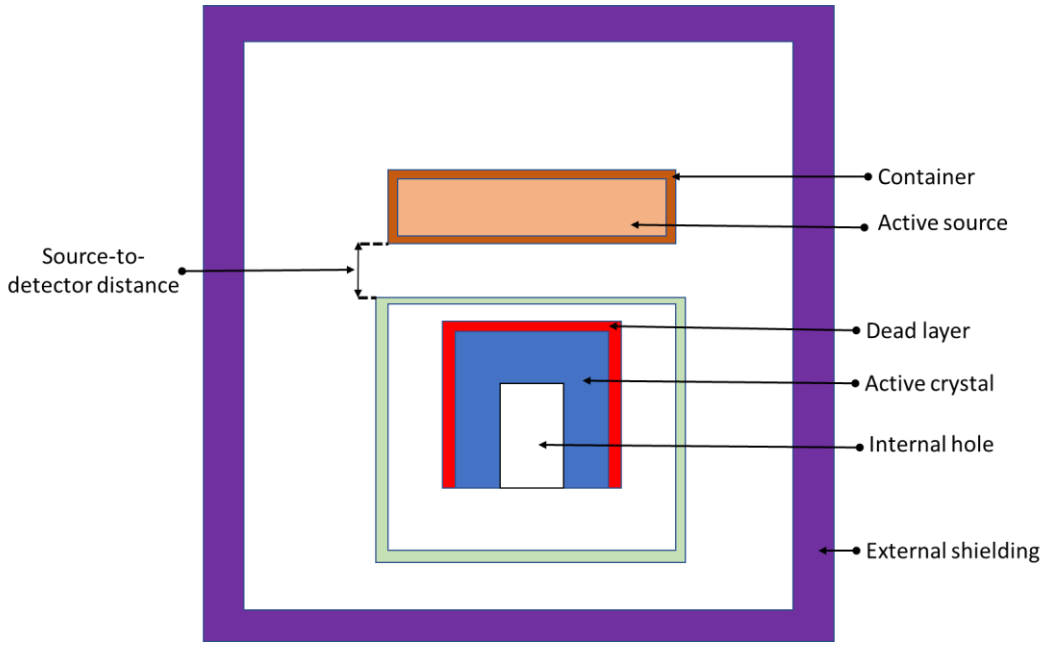

Figure 2: Typical experimental arrangement including a volume source and a detector installed in a shielding

For the practical use, several basic shapes are pre-defined in PUFI:

- Pure cylinder
- Basic detector (cylinder with a hole and dead layer)

- Container (full or partially filled)
- Housing (it can be used either for the detector cap or for the external shielding)
- Marinelli container

The main windows of PUFY is presented in Figure 3. To prepare the geometry file, you have to select the basic shapes and, for each one, to provide a few characteristic dimensions. The first step consists in defining the detector (crystal and dead layers dimensions) and its position relative to the reference plan. This is obtained by clicking on “Add geometry” and selecting “detector” in the list of pre-defined geometrical shapes.

The basic detector includes three parts: the internal hole, the active crystal and the front dead layer. The dialog window displayed in Figure 4 includes a rough visualization of the requested dimensions and allows to specify which element is the “active body” (in most of case, this is the crystal active volume) and the materials (numbers) of the different elements. (These material numbers are correlated with the ordered list of materials in the input file). Coming back to the main window, the user can input all the characteristic dimensions. At any time, the user can generate and visualize the generated PENELOPE geometry file.

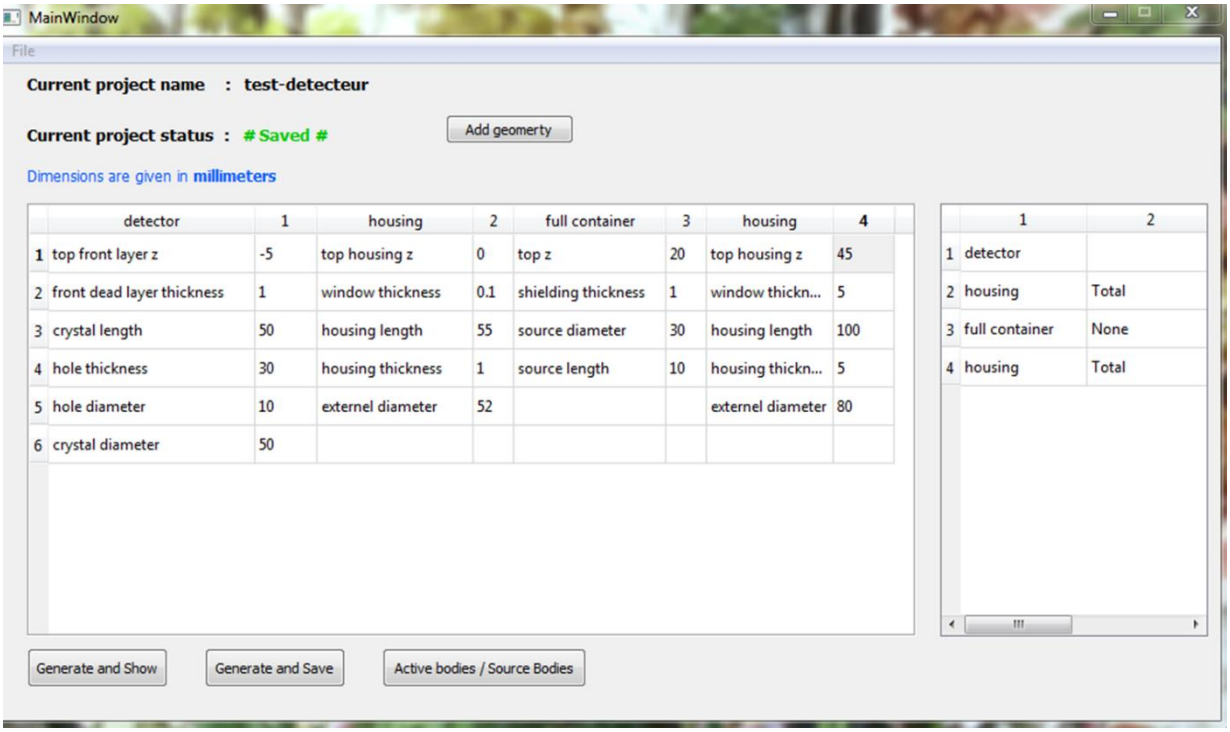

Figure 3: Main window of PUFI

Once all the elements are defined, the user can generate the PENELOPE geometry file and save it by clicking on “Generate and save” in the main window. For its practical use with PENELOPE, it can necessary to use the PenGeomJar application which allows renumbering the different elements in sequential order, using the “Relabel” option, as well as visualizing the defined geometry.

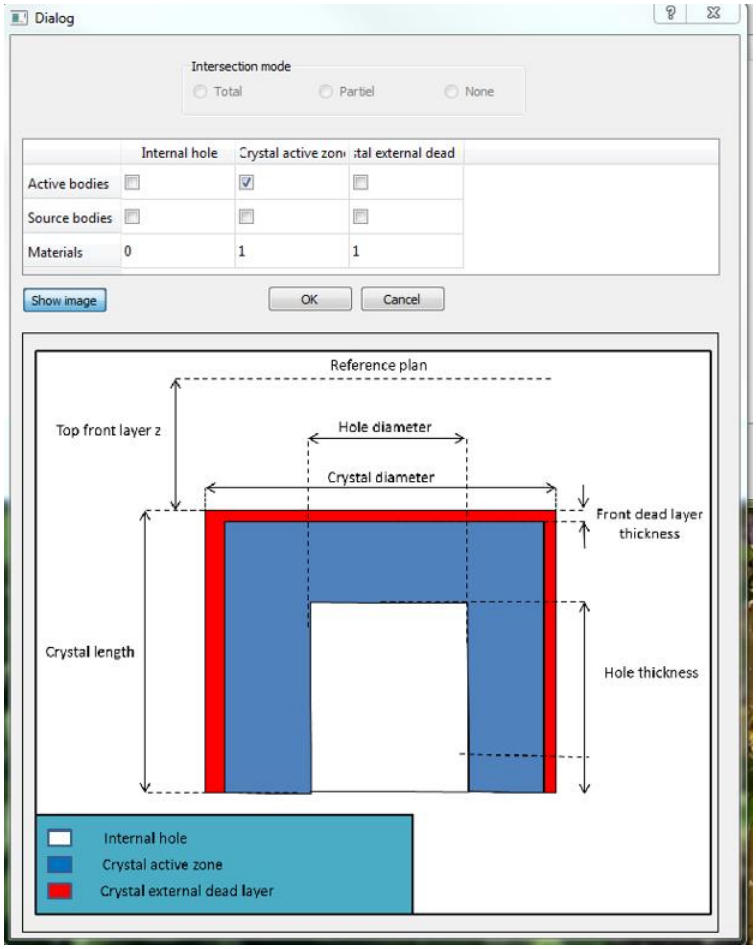

Figure 4: Dialog window to specify the characteristics of the geometrical elements (case of the detector)

4. Case of rounded detector

To improve the modeling of the detector, the roundness of the crystal entry face must be taken into account, which can be modeled as the intersection of a torus and a cylinder.

The general torus equation is:

$$\left(\sqrt{x^2 + y^2} - R^2\right)^2 + z^2 = r^2$$

where

R is the distance between the axis of the cylinder and the center of the torus,

r is the radius of the revolution circle generating the torus.

However, this equation is not quadratic and therefore cannot be directly modelled by PENELOPE. To overcome this difficulty, it was chosen to use an approximation method to model the rounding using several cones that can be described by quadratic equations. Figure 5 shows the projection on the plane (y,z) of the intersection of five cones and a cylinder. This structure is included as “rounded detector” in the list of basic shapes.

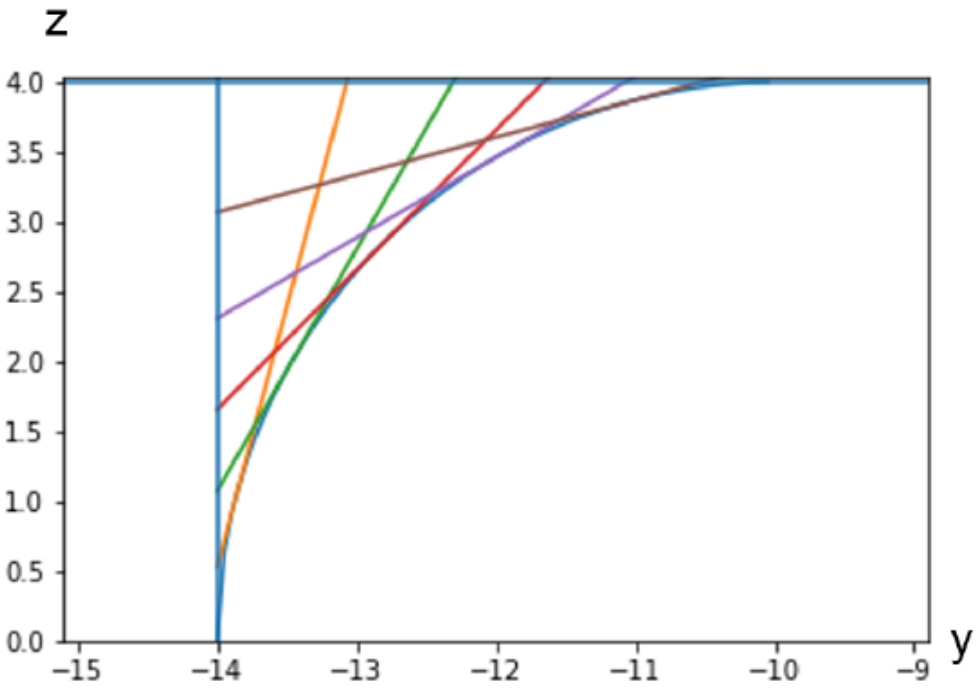

Figure 5: Approximation of a torus using the intersection of five cones and a cylinder

5. Conclusion

PUFI provides a fast and easy mean to prepare simple PENELOPE geometry files, what should be helpful for the training of new users. The software is available on the LNHB website, together with geometry example files and the user’s manual. Some example geometries are taken form the ICRM GSWG Monte Carlo exercise (Lépy *et al.*, 2019), and include two types of detectors and three types of volume sources. The cases of Marinelli container and volume source with an absorbing screen are also included. From these prepared geometries, it is very

easy to modify some dimensions directly in the main window to generate new cases: this can be useful to test the influence of changing the dimension of the source or the dead layer thickness, etc. As part of the increasingly frequent use of Monte Carlo simulation, PUFI brings a simple approach to optimize experimental conditions in gamma-ray spectrometry.

References:

Almansa, J., Salvat-Pujol, F., Díaz-Londoño, G., Carnicer, A., Lallena, A.M., Salvat, F., 2016. PENGEOM -A general-purpose geometry package for Monte Carlo simulation of radiation transport in material systems defined by quadric surfaces, Computer Physics Communications 199, 102-113. (https://doi.org/10.1016/j.cpc.2015.09.019)

Lépy, M.-C., Thiam, C., Anagnostakis, M., Galea, R., Gurau, D., Hurtado, S., Karfopoulos, K., Liang, J., Liu, H., Luca, A., Mitsios, I., Potiriadis, C., Savva, M.I., Thanh, T.T., Thomas, V., Townson, R., Vasilopoulou, T., Zhang, M., 2019. A benchmark for Monte Carlo simulation in gamma-ray spectrometry. Submitted to Applied Radiation and Isotopes

Salvat, F., 2015. PENELOPE-2014: A code System for Monte Carlo Simulation of Electron and Photon Transport, OECD/NEA Data Bank, NEA/NSC/DOC(2015)3. Issy-les-Moulineaux, France. Available from (http://www.nea.fr/lists/penelope.html)

Salvat, F., Fernández-Varea, J. M., 2009.Overview of physical interaction models for photon and electron transport used in Monte Carlo codes. Metrologia 46, S112–S138.