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An intercomparison of Monte Carlo codes used in gamma-ray spectrometry

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Abstract

In an intercomparison exercise, the Monte Carlo codes most commonly used in gamma-ray spectrometry today were compared with each other in order to gauge the differences between them in terms of typical applications. No reference was made to experimental data; instead, the aim was to confront the codes with each other, as they were applied to the calculation of full-energy-peak and total efficiencies. Surprising differences between the results of different codes were revealed.
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1. Introduction

In gamma-ray spectrometry, detector efficiency calibration represents a subject of considerable interest and importance, since it is always required for the analysis of a sample unless a standard with exactly the same characteristics is available. Monte Carlo simulations can be of significant help in the process of efficiency determination and their use has been gaining popularity over the years. Sophisticated codes are available nowadays, which incorporate accurate simulation of diverse interaction mechanisms of photons and electrons with matter and advanced ways of tracking the particles through the model of the measurement setup. Their applicability to and usefulness for the field of gamma-ray spectrometry has been firmly

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established, but a study of the intrinsic differences they possess has not been conducted yet. The differences between the packages and their modes of operation give rise to differences in the computed efficiencies even if exactly the same sample-detector model is fed to them. These differences can be treated as intrinsic uncertainties of the Monte Carlo approach in gamma-ray spectrometry, and they appear due to different approaches to particle tracking and the nuclear and material data used for it in individual packages.

The aim of the intercomparison exercise was to assess these uncertainties and as such the exercise did not involve any reference to the experimental data. Instead, it simply confronted the codes with one another, as they were applied to the calculation of full-energy-peak and total efficiencies for a precisely defined and very schematic model of a HPGe detector and the sample. Due to the absence of reference experimental data, the codes were thus only tested for their mutual compatibility and not for their absolute performance. The results of the exercise were meant to provide useful information for future intercomparison exercises involving the application of Monte Carlo codes to efficiency transfer and coincidence summing correction calculations and general guidelines for the intrinsic uncertainty that may be assigned to such results.

2. Method

Nineteen different laboratories participated in the exercise and seven different computer codes were used. Four codes were used by more than one participant: GEANT3 (Brun et al., 1987) (3 users), GEANT4 (Agostinelli et al., 2003) (5 users), PENELOPE (Salvat et al., 2006) (7 users) and MCNPX (McKinney et al., 2006) (3 users). The codes GESPECOR (Sima et al., 2001), EGS4 (Nelson et al., 1985; Kawrakow and Rogers, 2006) and TRIPOLI-4 (Both et al., 2003) were all used by one participant only. Some participants used more than one code. Two different rounds of simulations were carried out, as discussed in more detail below. The results presented in this work refer to the second and decisive round.

GEANT3 was employed by all of its three users as version 3.21. One single version (8.0) of GEANT4 was also used, but with different input data, namely with the default set, the set specifically designed for low energies, and the set identical to the data used by PENELOPE. PENELOPE itself was employed in several versions, numbered by the year of publishing of the code, which ranged from 2001 to 2005. One user applied the MCNP code and two others the latest MCNPX version, while EGS4 was used both in its original version, as well as in its latest EGSnrc variant. GESPECOR and TRIPOLI-4 were both employed in their latest versions.

The participants were asked to calculate full-energy-peak and total efficiencies for three different sample-detector geometries. In all of them, complete cylindrical symmetry of the sample-detector arrangement and geometry was presumed. The first arrangement (Geometry #1) consisted of a bare germanium crystal ($60 \times 60\,mm^2$, density $5.323\,g\,cm^{-3}$) and a point source located 10 mm from the crystal surface and on its symmetry axis. In the second setup (Geometry #2) the source remained the same, but the most important parts of a real HPGe detector have been added to the detector model, namely, the dead layer, the central hole and the aluminium housing. Geometry #3 (Fig. 1) was geared towards testing the possible differences in the treatment of the sample, as the point source was replaced by a cylindrical extended source containing a liquid solution, with the detector model remaining the same as in Geometry #2. The sample density was set to $3.0\,g\,cm^{-3}$, with the intention of verifying proper self-absorption correction calculation by the codes in relatively demanding conditions. The fact that the detector model used in the second and the third geometry was the same made it possible to define Geometry #4 as a ratio of the results of Geometries #2 and #3. This procedure is of interest in the efficiency transfer method, often used for the calculation of full-energy-peak efficiencies, since any inadequacies in the simulation of both original geometries should cancel out to a large extent.

The energies for which the efficiencies were to be calculated were selected from the point of view of the

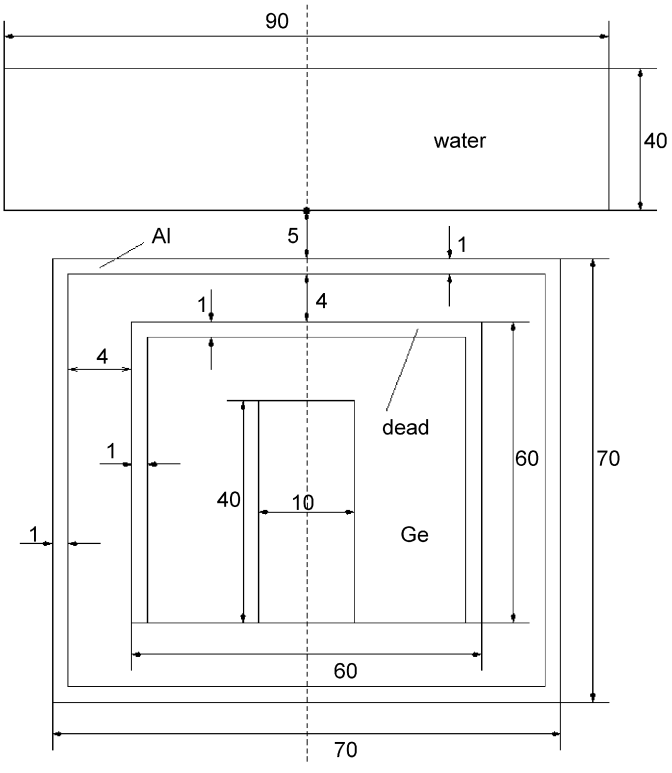

Fig. 1. Geometry #3. The germanium crystal has the same dimensions and density as in Geometry #1 ($60 \times 60\,mm^2$, $5.323\,g\,cm^{-3}$), but has a 1 mm top dead layer and 1 mm side dead layer. A central hole is also drilled into the back side of the crystal, which is encased in aluminium housing. The point source of the first two geometries is replaced by an extended source in the form of a water cylinder with an artificial density of $3.0\,g\,cm^{-3}$. All dimensions are given in millimeters. The drawing is not to scale.

general characteristics of the efficiency curve in gamma-ray spectrometry, rather from the point of view of pure interaction of gamma-rays with matter. That is to say, since the efficiency curve bends at around 120 keV in the log–log scale for p-type detectors, we decided to make the energy grid denser around this value in the first round and sparser at higher energies where the curve is known to follow an approximately straight line. The lowest energy of 45 keV was added to the list, since it is of interest for Pb-210 activity determination in environmental samples. In the first round, the energies selected were 45, 60, 80, 100, 120, 140, 160, 300, 500, 1000, 2000 and 3000 keV. This set was reduced in the second round to 45, 60, 120, 200, 500 and 2000 keV, in order to shorten the calculation time. Additionally, some participants also submitted results for the energy of 200 keV. In the second round, only sample-detector geometries 2, 3 and 4 were considered. In both rounds, all the codes except for TRIPOLI-4 employed the tracking of both photons and electrons.

The relative statistical uncertainties of all the results were required to be kept at 0.1% in the first round of calculations, since minimal differences between the obtained results were initially expected. As this turned out not to be the case, the condition was relaxed to 0.3% in the second round, in order to speed up the calculations.

3. Results and discussion

In some cases, the results of the first round of calculations revealed differences in excess of 10% between the median value of the efficiency within a group of users that all employed the same code and the individual outliers. This was deemed unacceptable and inexplicable by possible differences between the different versions of the same code. The problem did not occur with Geometry #1, but it was present with other geometries. Small working groups of users of the same code were then established and a coordinator selected for each of them. The essential unifiying measures introduced in the second round of calculations were the following:

- No variance reduction techniques were allowed to be employed.
- A unified set of control parameters for the individual code was selected within each user group and applied by all its users.
- An energy cutoff of 1 keV was adopted for the tracking of particles with all the codes except in GEANT3, which has a built-in cutoff of 10 keV.
- A unified definition of the full-energy-peak was adopted—a spectrum of exactly 1000 channels was required for each simulated energy, with channel 1000 corresponding to this energy.

The ideal full-energy-peak area definition would have been the most physically sound one, according to which all events that result in the full deposition of the initial photon energy in the active part of the detector crystal should simply be counted. However, its direct implementation was deemed impractical for some of the codes and the imperative was to find a universal definition which would enable comparison between the different programs. The adopted 1000-channel definition is of general practical use and avoids the typical pitfalls, such as using a fixed number of channels along with a fixed relation between energy and channel number, which easily results in too few channels being actually used with low-energy photons.

With the above-listed criteria set, round two of the calculations was initiated for a reduced set of energies and geometries. The results of the second round are satisfactory as far as the uniformity of results within a single group is concerned. With a few exceptions, the differences within each code have been reduced to values smaller than 1% for all the geometries and all the energies. The notable exceptions are the Standard Physics data set for GEANT4 at lower energies and one particular case of the use of the PENCYL mode of operation of PENELOPE at higher energies. The reason could lie in different interaction cross sections in the case of Standard Physics, but it is not clear what it may be in the PENCYL case, since it appears that other users applied this code too. These difficulties are not present, however, for the ''relative'' Geometry #4.

With the results supplied by different users of the same code satisfactorily unified, one was able to study the (relative) differences between the median results of different codes. These are shown in Figs. 2–4. The first two of these figures depict the results of GEANT3, GEANT4, MNCP and PENELOPE (code group A), while the last figure illustrates the computations done with EGS, TRIPOLI-4 and GEPSECOR (Code Group B). For each of the codes and for each of the energies, a median was calculated over all the different users' values. A grand median was then calculated with regard to the code group A codes. The figures show the energy dependence of the relative differences between the medians of the individual codes and the grand median. The figures only depict full-energy-peak efficiencies, but a very similar relationship also exists for total efficiencies in general. Fig. 2 shows the results of code group A for Geometry #3, but a very similar picture emerges for Geometry #2. Similarly, the results of code group B for Geometry #2 are quite close to those for Geometry #3 of the same group. Geometry #4 yields similar results for both code groups, although those for code group B are less favourable.

For code group A, it can be concluded that the differences between the individual codes are quite striking for geometries #2 and #3 at lower energies and were not expected to be so pronounced prior to the exercise. On the other hand, the agreeement is satisfactory for the ''relative'' Geometry #4. In Geometries #2 and #3, the results of GEANT3 and MCNP on the one hand and those of PENELOPE and GEANT4 on the other hand seem to be similar. The two latter programs have been developed more recently than the former pair and it may be that they

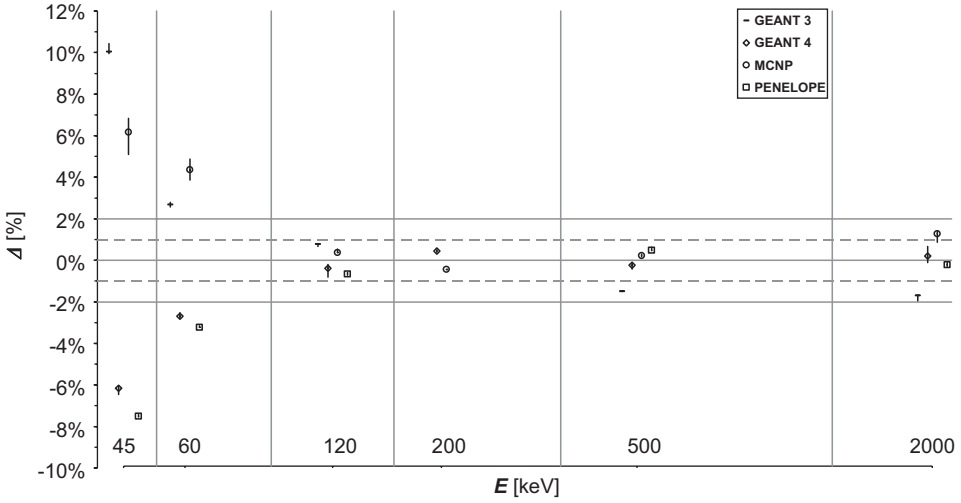

Fig. 2. Geometry #3, code group A. The relative differences Δ between the grand-median full-energy-peak efficiency and the medians of the individual codes at different gamma-ray energies E (see text). The variability between users within each code is displayed with vertical bars representing the interquartile range (IQR).

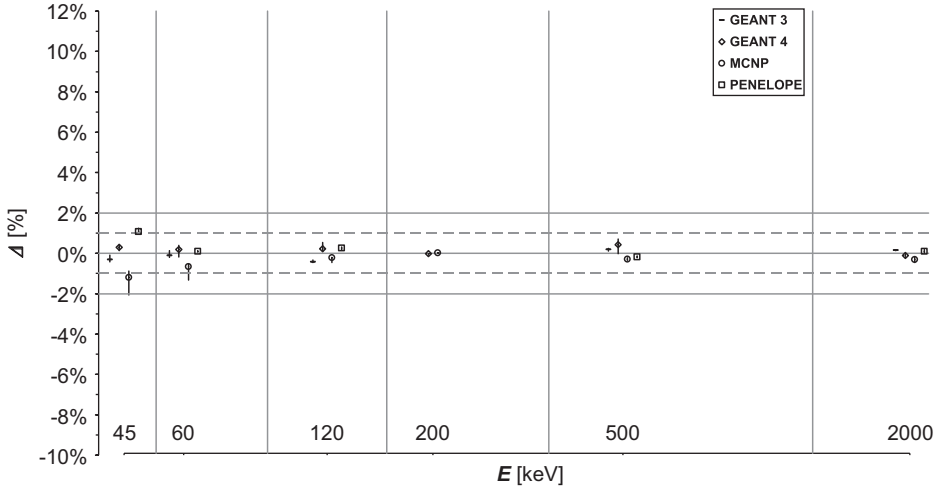

Fig. 3. Geometry #4, code group A: Same as Fig. 2.

incorporate different physics and above all different cross sections than the older two. One also notices that the results of code group B show a similar dependence of those of code group A at lower energies, if in the latter group the results of GEANT3 and MCNP are ignored. These features remain to be investigated in full, but at least in the case of GEANT3 a possible explanation has been offered by Decombaz et al. (1992), who noticed that in their data the systematic bias between experimental and calculated full-energy-peak efficiency below 150 keV "is explained by the fact that for low energies the cross sections calculated by GEANT3 appreciatively differ from those found in the literature…". The 10 keV built-in cutoff for particle tracking in GEANT3 also results in incomplete treatment of germanium X-ray escape probabilities at low energies.

The fact that in code group B the result of TRIPOLI-4 stands out at the highest energy (Fig. 4) can probably be attributed to the fact that the simulation of the electron transport was switched off in this code.

In general, one can say that at present a relative use of any of the Monte Carlo codes (Geometry #4) produces the most reproducible results. In any other mode of operation, the same detector model might yield different results with different simulation codes. This also means that a detector model, the parameters of which have been optimized in order to match a set of experimental data, is inextricably linked to the code with which this procedure has been carried out. A different code might not be able to reproduce the measured values with such a model.

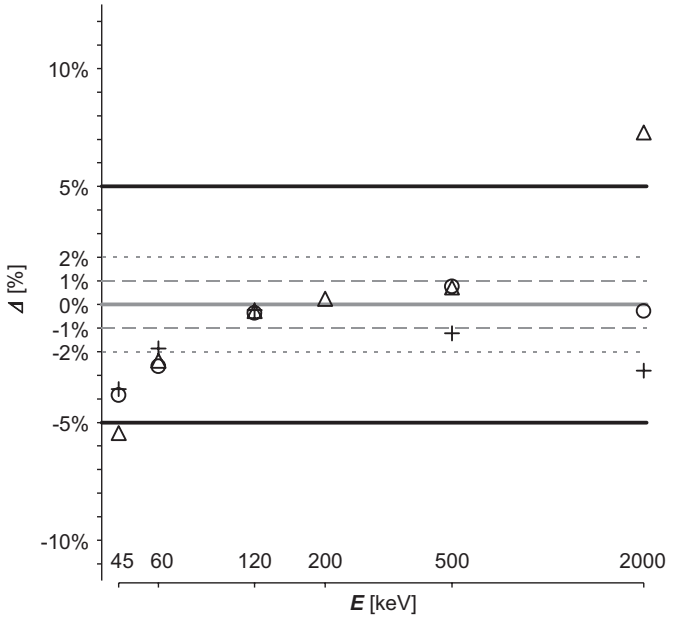

Fig. 4. Geometry #2, code group B. Same as Fig. 2. Symbols: cross—GESPECOR, circle—EGS4, triangle—TRIPOLI-4.

4. Conclusion

A study of the most commonly used Monte Carlo codes in gamma-ray spectrometry has been conducted to see how much the results of different codes differ from each other when full-energy-peak and total efficiencies are computed for well-defined sample-detector arrangements. While it was possible, after some initial difficulties, which emphasized the importance of the definition of the full-energy-peak, to obtain uniform results from different users of the same code and to a large extent from different versions of the same code, the differences between the different codes themselves turned out to be suprisingly large, reaching 10% in some cases at lower energies (45 keV). The reasons for these discrepancies remain to be investigated. More favourable results can be expected at higher energies in general and when the codes are used in the (relative) efficiency-transfer mode in particular, with the diffrences reduced to 1%. The statistical uncertainties of the calculated efficiencies were kept at 0.3%.

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