Nuclide++: A C++ module to include DDEP recommended radioactive decay Data in Geant4

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NUCLIDE++: A C++ MODULE TO INCLUDE DDEP RECOMMENDED RADIOACTIVE DECAY DATA IN GEANT4

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Abstract

This article describes the Nuclide++ module developed at LNE-LNHB to simulate the decay schemes related to single or multiple radionuclides, by randomly selecting decay pathways. Written in C++, with respect of the Geant4 coding style, this module can be used transparently in Geant4-based simulation applications as an alternative to the existing Radioactive Decay Module (RDM). Nuclide++ takes advantage of the DDEP recommended data, accurate β-emitting spectra calculation and detailed description of the atomic rearrangement. This module can be useful in many applications, especially those involving radioactive sources. The reliability of the module was verified through comparisons with a while chosen radionuclides.

Keywords: Radioactive decay, DDEP data, Geant4 simulation.

1. Introduction

In a wide range of radioactivity measurements, it has become common practice to investigate the response of detectors by the means of Monte Carlo (MC) simulation codes. In most of these tools, as for instance Geant4 code (Agostinelli et al., 2003; Allison et al., 2006), the simulation of radioactive decay represents an important task. Thus, a comprehensive and accurate knowledge of radionuclides decay-scheme data is crucial. This is the case in the field of radionuclide metrology (Simpson and Judge 2007; Karam et al., 2015). For a long time, LNE-LNHB is involved in nuclear data evaluations and the dissemination of recommended atomic and nuclear values in the frame of the Decay Data Evaluation Project (DDEP, Kellett and Bersillon, 2017) involving several national metrology institutes (NMIs). The evaluated data are produced from published experimental results, completed if necessary with theoretical calculations. A dedicated database gathers these recommended data for more than 200 radionuclides, available on the LNHB website (*http://www.lnhb.fr/nuclear-data*) and also published in the BIPM Monographie-5 series (Bé et al., 2016).

Recently, a Fortran subroutine for radioactive decay, PENNUC, using the DDEP database (exported in a specific input file format) has been developed at CIEMAT in collaboration with LNE-LNHB (García-Toraño et al., 2017). This radioactive decay package can be used either independently to generate the particles resulting from the decay process or directly within the PENELOPE Fortran MC code (Salvat, 2015). In the same approach, an equivalent tool written in C++, named Nuclide++, specially designed to work with the Geant4 code, is presented in this paper. This module aims at simulating the complete decay chain of a given radionuclide by randomly selecting all the decay pathways following a disintegration, using recommended data from DDEP (half-life, nuclear level structure for parent and daughter nuclides, branching ratios, evolution time of radiation, type and energy of particles etc.). It also takes into account the nuclear de-excitation of subsequent daughters following the same disintegration event, as well

as the metastable levels presenting lifetimes longer than a threshold set by the user. This permits the dead-time effect to be considered, for example, due to the resolution time characterizing the detection system (useful in photon spectrometry simulation applications). The initial energies of electrons and positrons in the case of β-emitting radionuclides are sampled from spectra calculated with the BetaShape program, developed at LNE-LNHB for improving nuclear data related to β emission proprieties (Mougeot, 2015). The de-excitation cascade *i.e.,* the set of successive transitions that occurs from an initial vacancy, is sampled using the transition probabilities provided by the Lawrence Livermore National Laboratory (LLNL) - Evaluated Atomic Data Library (EADL) (Perkins et al., 1991).

The objective of this work is to propose to the Geant4 users the possibility to perform simulations with DDEP recommended data and a more detailed decay model, as an alternative to the existing Radioactive Decay Module (RDM) available in Geant4. The simulation model in this original module depends on nuclear data taken from the Evaluated Nuclear Structure Data File (ENSDF).

The reliability of the new module (Nuclide++) in terms of coincident particle cascades generated during a disintegration event, is shown through comparisons with the PENNUC package (available in the PENELOPE code) and the Geant4-original RDM, for chosen radionuclides with complex decay schemes.

2. Short description of Geant4

2.1 Implementing an experiment with Geant4

The use of Geant4 software is now widespread for radiation transport calculations, in a large variety of domains such as nuclear and accelerator physics, space physics or medical applications. Users can find an exhaustive range of physics models, a large set of particles over

a wide energy range and a diversity of tools (for defining geometries, modelling radiation sources, detection systems, and analyzing results), to simulate experiments. Written in C++, the object-oriented coding style and the exploitation of advanced software engineering allow the user to easily integrate an additional module or extend an existing one, without disrupting the basic structure of the code. Therefore, users can call on a set of C++ classes to describe their proper classes, which in turn will be called by the main program. As for instance, the geometry of an experiment (in terms of volume and filling material, physical and optical properties) is described in *MyDetectorConstruction* class; particles, interaction processes and physical models are defined in *MyPhysicsList* class; and the generation of primary particles (type, energy, position and direction) is defined in *MyPrimaryGenerator* class. A main program ensures the link and brings together basic Geant4 classes with mandatory and optional classes by calling in turn, each describing a specific stage of the simulation. Fig. 1 shows an example of a classic configuration of the Geant4 simulation model.

2.2 Existing radioactive decay in Geant4

The simulation of radioactive decay consists in processing the spontaneous transformation of an atom with an unstable nucleus into daughter nuclides, left in the ground state or an exited state, and generating the resulting products *i.e.*, β, γ and α-emission, neutrinos and conversion electrons, including the de-excitation of the daughter atom involving the production of X-ray and Auger electrons. Since the version 2.0, a module for the simulation of radioactive decays is available in Geant4, based on the original work of Truscott et al. (2000) and Truscott (2002). Decay processes are treated in the *G4RadioactiveDecay* and associated classes, exploiting the evaluated data from ENSDF (Tuli, 1996; Hauf et al., 2013). The module is completed and updated through the different released versions. The demonstrative examples of radioactive decay and the use of some features (named *rdecay01* and *rdecay02)* are available in the repository of extended-examples of Geant4.

3. Description of the Nuclide++ module

Nuclide++ functionalities are implemented in a C++ class: *DDEPNuclideDecay.cc* and associated header class *DDEPNuclideDecay.hh*. This contains different functions to read the nuclear data for a chosen radionuclide, randomly select decay pathways and generate the emitted particles. The *DDEPNuclideDecay.cc* class should be set as a sub-class of Geant4 user class: *MyPrimaryGeneratorAction*, in which a user has to specify the generation of primary events. Nuclide++ is then processed in the *GeneratePrimaries()* function called at the beginning of each event (Fig. 1). An environment variable, *G4DDEP_DATA,* must be set to point to the path of the radionuclide data files (extracted from the DDEP database).

3.1 Query data and sampling decay pathways

The first task concerns reading and storing the data from the DDEP database, carried out in the function *ReadNuclideData()* with the following entries in arguments: *i*) name of the radionuclide of interest; *ii*) the decay-extension factor (0 to follow instable nucleus, 1 to follow instable daughters); and *iii*) the resolution time (a characteristic of the detectors). The required nuclear data are loaded into associated variable types. The function then identifies the disintegration modes and normalizes branching ratios and transition probabilities. The particles released in each disintegration sequence are then obtained randomly through two loops: the branching loop and the transition loop using a binomial trial with normalized probabilities.

The particles resulting from delayed transitions are selected considering the time evolution of radiations, obtained from an exponential distribution using the expected lifetimes of the excited levels. If the lifetime of the transition level exceeds the input resolution time, the level is treated as metastable and the subsequent released particles are not retained in the ongoing disintegration event. When the decay-extension factor is set higher than zero, instable daughters are subsequently treated in the same disintegration event.

3.2 Beta emission processing

In simulations involving radioactive sources, as for instance in ionizing-radiation metrology, the emission probability of the β particles (a continuous spectrum from null energy to the transition energy) is also crucial. Obviously mean energies directly depend on the shape of β spectra and on the nature of the transition according to the structure of the nuclear states involved.

In this work, Nuclide++ takes advantage of relevant assumptions and calculation methods carried out in the BetaShape code (Mougeot, 2017), officially adopted for decay data evaluation by the DDEP collaboration. In the first version of this code, the relativistic electron wave functions are determined by numerically solving the Dirac equation for a Coulomb potential from a uniformly charged sphere. From these wave functions, allowed and forbidden unique transitions of any order can be calculated accurately while forbidden non-unique transitions, which are very sensitive to nuclear structure, are still estimated using the ξ approximation. The main features of this code include: *i*) a database of experimental shape factors; *ii*) the provision of mean energies and logft-values, as well as beta and neutrino spectra; *iii*) the ability to interface with ENSDF files; and *iv*) the propagation of uncertainties from input data. A detailed description is given in Mougeot (2015) and Mougeot (2017).

For a better efficiency of the Monte Carlo processing, the BetaShape code has been applied to every DDEP evaluation and a dedicated library has been created which gathers the beta spectra, ensuring the consistency with DDEP data. Therefore, the β spectrum of interest is read at the beginning of the simulation process and then for each primary event, the initial kinetic energy of an electron or a positron released from the β transition is randomly chosen within the accessible energies by carrying out a linear interpolation of the calculated spectra.

3.3 Atomic relaxation processing

The electron capture (EC) and internal conversion (IC) are the radioactive decay sequences causing atomic de-excitation. During the EC process, an inner orbital electron, generally K- and L-shell electrons, is captured by the nucleus. This leads to the transformation of a proton into a neutron and the atomic number is reduced by one unit, simultaneously accompanied by the emission of a neutrino. The IC process occurs alternatively to γ-emission (when an excited nucleus returns to its ground state or intermediate excited levels) by transferring its excitation energy to an X-shell electron (K, L, M and N), which is ejected from the atom, leaving it in an excited state. The electron carries a discrete fraction of the decay energy. Since there is no transformation of the nucleus, the atomic number and atomic mass number remain unchanged. In both cases, the atom is in an excited state *i.e.*, with a vacancy in its electronic structure. The relaxation towards the ground state occurs through a sequence of radiative and non-radiative transitions. In the first case, the vacancy is filled by an electron from an outer sub-shell and an X-ray with characteristic energy is released (fluorescence effect). In the second case, the vacancy is filled by an outer electron and the excess energy is released through the emission of an electron from a further subshell (Auger effect).

The atomic de-excitation cascade products are sampled using relaxation data of elements obtained from a specific database containing possible transitions, transition probabilities and energies of the emitted X rays or electrons for ionized atoms with a single vacancy in the K shell or in an L, M or N subshell. This database is prepared using the radiative and non-radiative transition probabilities for sub-shells of elements extracted from the LLNL EADL (Perkins et al., 1991). The energies of X-rays resulting from shell vacancies were taken from Deslattes et al. (2003); Bearden (1967); Bearden and Burr (1967).

The Nuclide++ routine transcribes the atomic rearrangement on the basis of the detailed $KL_1L_2L_3$, M, N, model which is adequate for EC radionuclide simulations (Grau Malonda et al., 1999; Kossert and Grau Carles, 2006). The rearrangement model includes L–Coster–Kronig

emission and detailed sampling of L_i-subshell energies, L-Auger electrons and L-X-rays, instead of using averaged values.

3.4 Interfacing with Geant4

For each generated event, the Nuclide++ routine returns a matrix containing the initial-state variables of particles released in a disintegration event. This matrix contains the event ID (matching with G4Event ID), the particle type (α, γ, X-ray, electron or positron), the associated energy, the parent ID and the transition ID. The initial positions (that of the active nucleus) and the directions of particles are determined from classical methods in Geant4. The matrix is then passed to tracking through the basic *G4ParticleGun* class, which shoots one primary particle of a given energy from a given point at a certain time in a given direction (*http://geant4.web.cern.ch/support/user_documentation* (Chapter 2); Allison et al., 2016).

4. Verification of Nuclide++ module

The code implementations have been verified for consistency with DDEP data by comparing with the PENNUC package developed at CIEMAT and working with the PENELOPE code (García-Toraño et al., 2017). Since PENNUC is well validated and considered in the radionuclide metrology community as a reference, comparison against it provides a valuable evaluation. Simulated cascades of particles were produced with 10^6 decays of the chosen radionuclides and stored in output files. Comparisons were then carried out through different histograms. In the case of Geant4, a simple simulation was performed with the version geant4.10.1 and 10^6 decays of the chosen radionuclides within an otherwise empty geometry.

4.1 γ-transition emissions

The reliability of intensities and energies released in γ-transitions is shown in the case of two radionuclides with complex decay-schemes incorporating coincident photon transitions:

^{152}Eu and ^{133}Ba. Fig 2 shows the simplified decay scheme of both radionuclides drawn from the *Nucléide - Lara* application (*http://www.lnhb.fr/nuclear-data/module-lara*).

^{152}Eu disintegrates by electron capture (~72.1%) and by positron emission (~0.03%) to ^{152}Sm, and by beta minus emission (~27.9%) to ^{152}Gd. Fig. 3 shows the γ and X-ray emissions from simulated cascades; the resulting intensities are reported in Table 1. To check the consistency between Nuclide++ and both PENNUC/Geant4-RDM, a z-score test was applied to the released particle-energy intensities. This test consists of calculating the difference $d = |c_1 - c_2|$ between the counts c_1 and c_2 of the X-ray– or γ– energies released and the associated uncertainty: $u(d) = \sqrt{u^2(c_1) + u^2(c_2)}$. If $\frac{d}{u(d)} < 1$ then results are consistent.

The same comparison is also reported in Table 2 for ^{133}Ba, which disintegrates by EC mainly to two ^{133}Cs excited levels of 437 keV (~85.4%) and 384 keV (~14.5%), and with three minor branches (<1%) to the 161 keV and 81 keV exited levels and to the ground state.

4.2 β-transition emissions

For β^+ emitting nuclides, the reliability of Nuclide++ was verified with some radionuclides of particular interest in nuclear medicine: the short-lived PET radionuclides ^{11}C and ^{18}F, and the long-lived PET radionuclide ^{44}Sc.

^{11}C disintegrates by 99.75% β^+ and 0.25% by electron capture to the ground state of the stable ^{11}B. Fig. 4 compares the histogram obtained with Nuclide++ to PENNUC and Geant4-RDM for ^{11}C with 10^7 decays. As Nuclide++ and PENNUC routines use the same data and the same

prohibition factors derived from measured spectra (Mougeot, 2015), resulting spectra are in very good agreement, as are the respective maximum and average energies, see Table 3, where the variation of the average energies is lower than 0.3%. For Geant4-RDM the average energy is about 3% lower.

In the case of ^{18}F which decays 96.86% by β^+ and 3.14% by electron capture, the average energy obtained with Geant4-RDM is about 7.6% lower.

The Nuclide++ module was also verified with the pure β^--emitting radionuclides ^{63}Ni, ^{90}Y and ^{32}P; the maximum and average energies are also reported in Table 3.

5. Conclusion and comments

In this present work, we have described a C++ module (Nuclide++) for the simulation of the decay scheme of a given radionuclide based on recommended DDEP data. The module simplifies physical processes of the radioactive decay to generate only the particles associated to the spontaneous emission of ionizing radiation: α-, β- and γ-emissions, and X-ray and Auger electron emissions from the atomic rearrangement. Nuclide++ allows simulating radioactive sources containing a compound of radionuclides, including the simulation of decay chains and the time dependence of detectors (to account for the delay associated with metastable state decays in cascade processing). This radioactive decay module is designed to be used transparently in the Geant4-based simulation applications, as an alternative to the existing Geant4-RDM.

In general, very good agreement has been obtained with the PENNUC subroutine available in the electron-photon transport code PENELOPE for a variety of radionuclides. Comparing to the existing Geant4-RDM, the α and γ-emission intensities are consistent in the per-decay radionuclides tested. Significant consistency improvements have been verified especially in β-

emitting nuclides due to precise calculation of spectra offered by the pre-existing code BetaShape, and in atomic rearrangement induced by the electron capture process or internal conversion due to a detailed sampling of X-ray and Auger electron emissions. In the future, the Nuclide++ module will directly benefit from new and updated DDEP evaluations, from improvements of the BetaShape code, for which a new version is expected to be released soon with a more precise treatment of both beta and electron capture transitions, and future versions of the EADL atomic library, whose currently limited precision is becoming problematic for a wide range of applications.

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Highlights

- A C++ module to generate decay schemes of radionuclides with DDEP recommended data is presented.
- The module permits to efficiently simulate radioactive sources with single or multiple radionuclides.
- Efficiently process complete decay chains, including metastable levels and time dependence of detectors.
- The reliability is demonstrated through comparisons with chosen radionuclides.
- The module can be used transparently in Geant4-based simulation applications, alternatively to existing Geant4-RDM.

Figure captions:

Fig. 1: Diagram of Nuclide++ module implementing radioactive decay with DDEP data, showing the relation with Geant4 user classes.

Fig. 2: Decay schemes of ^{152}Eu and ^{133}Ba, taking from LARA web site.

Fig. 3: Comparison of γ and X-ray emissions from 10^6 ^{152}Eu decays, resulting from simulated spectra of Nuclide++, PENNUC and Geant4-RDM. The last two are shifted for better identification of peaks: +45 keV and +2 a.u. for PENNUC; +90 keV and +4 a.u. for Geant4-RDM.

Fig. 4: Comparison of β-emitting radionuclides spectrum generated: (a) ^{11}C (β^+-emitter) and (b) ^{63}Ni (β^--emitter).

Table captions:

Table 1: Energies and photon intensities of the main γ and X-ray emissions from 10^6 disintegrations of ^{152}Eu decays (sorted by intensity).

Table 2: Energies and photon intensities of the main γ and X-ray emissions from 10^6 disintegrations of ^{133}Ba decays (sorted by intensity).

Table 3: Maximum and average energies obtained from β-spectrum generated with the three radioactive decay modules.

Fig. 1

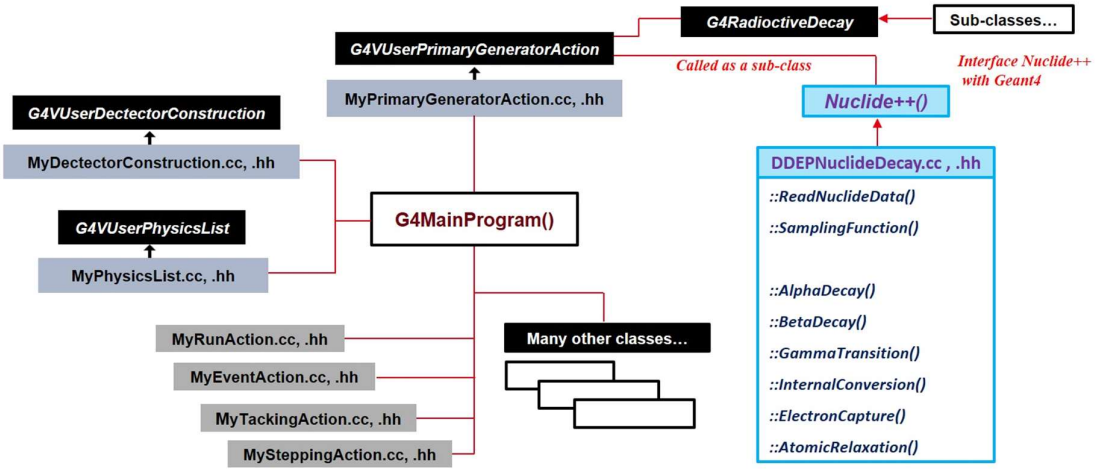
G4RadioctiveDecay
Sub-classes…
G4VUserPrimaryGeneratorAction
Called as a sub-class
Interface Nuclide++ with Geant4
MyPrimaryGeneratorAction.cc, .hh
Nuclide++()
G4VUserDectectorConstruction
MyDectectorConstruction.cc, .hh
DDEPNuclideDecay.cc , .hh
::ReadNuclideData()
::SamplingFunction()
G4VUserPhysicsList
G4MainProgram()
MyPhysicsList.cc, .hh
::AlphaDecay()
::BetaDecay()
::GammaTransition()
::InternalConversion()
::ElectronCapture()
::AtomicRelaxation()
MyRunAction.cc, .hh
Many other classes…
MyEventAction.cc, .hh
MyTackingAction.cc, .hh
MySteppingAction.cc, .hh

Fig. 2

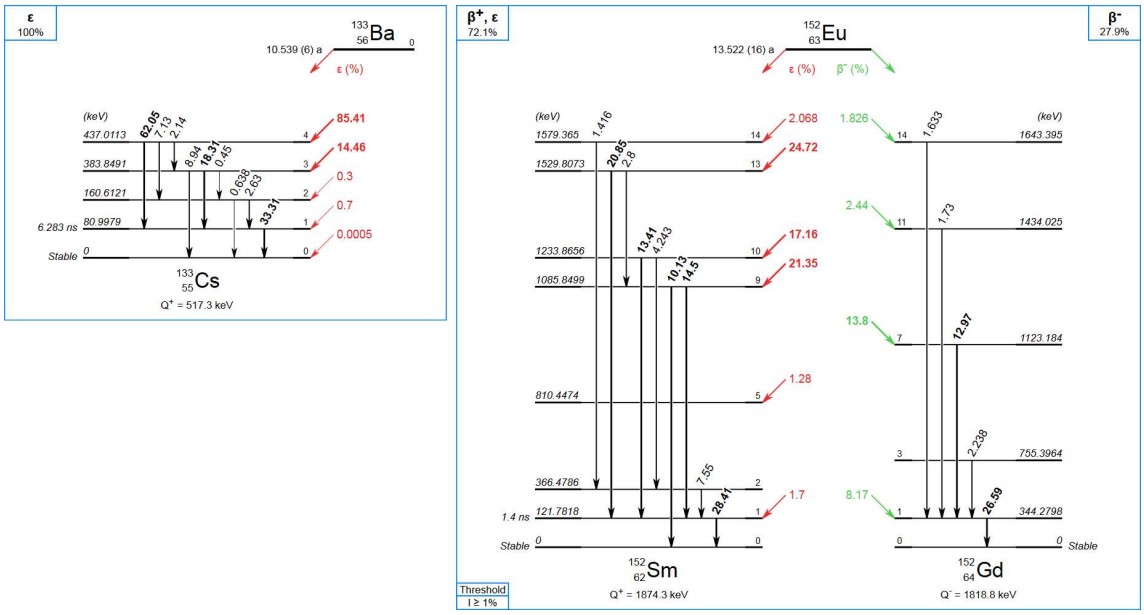
ε
100%
133 56 Ba 0
10.539 (6) a
ε (%)
(keV)
437.0113
383.8491
160.6121
80.9979
6.283 ns
0
Stable
62.05
7.13
2.14
8.84
18.31
0.45
0.638
2.63
33.31
85.41
14.46
0.3
0.7
0.0005
133 55 Cs
Q+ = 517.3 keV
β+, ε
72.1%
β-
27.9%
152 63 Eu
13.522 (16) a
ε (%)
β- (%)
(keV)
1579.365
1529.8073
1233.8656
1085.8499
810.4474
366.4786
121.7818
1.4 ns
Stable
1.416
20.85
2.8
13.41
4.243
10.13
14.5
7.55
28.41
2.068
24.72
17.16
21.35
1.28
1.7
152 62 Sm
Q+ = 1874.3 keV
1.826
2.44
13.8
8.17
1643.395
1434.025
1123.184
755.3964
344.2798
1.633
1.73
12.97
2.238
26.59
152 64 Gd
Q- = 1818.8 keV
Threshold
I ≥ 1%

Fig. 3

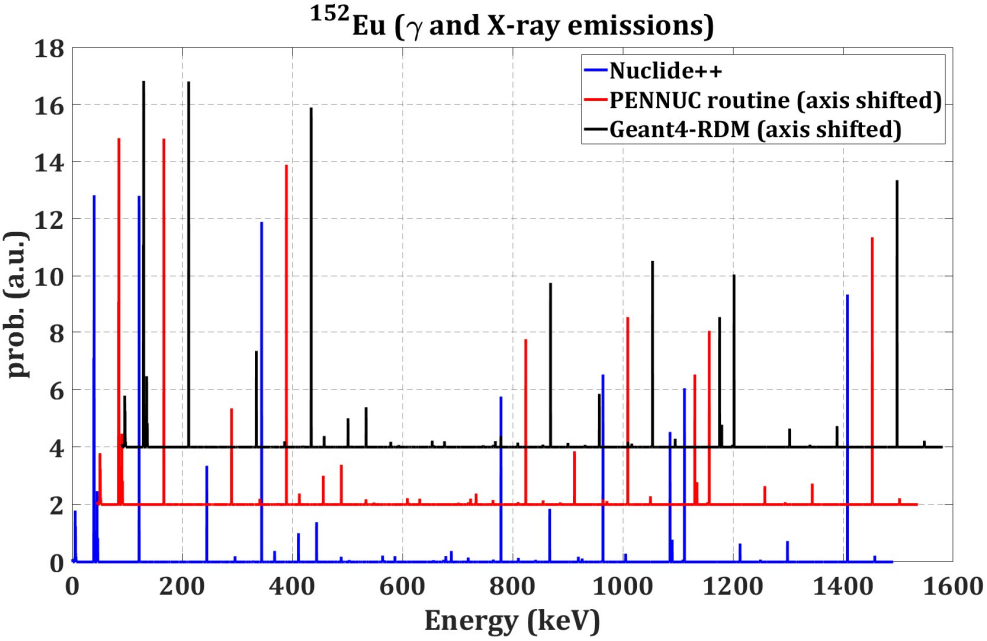
^{152}Eu (γ and X-ray emissions)
Nuclide++
PENNUC routine (axis shifted)
Geant4-RDM (axis shifted)
prob. (a.u.)
Energy (keV)
0
2
4
6
8
10
12
14
16
18
0
200
400
600
800
1000
1200
1400
1600

Fig. 4

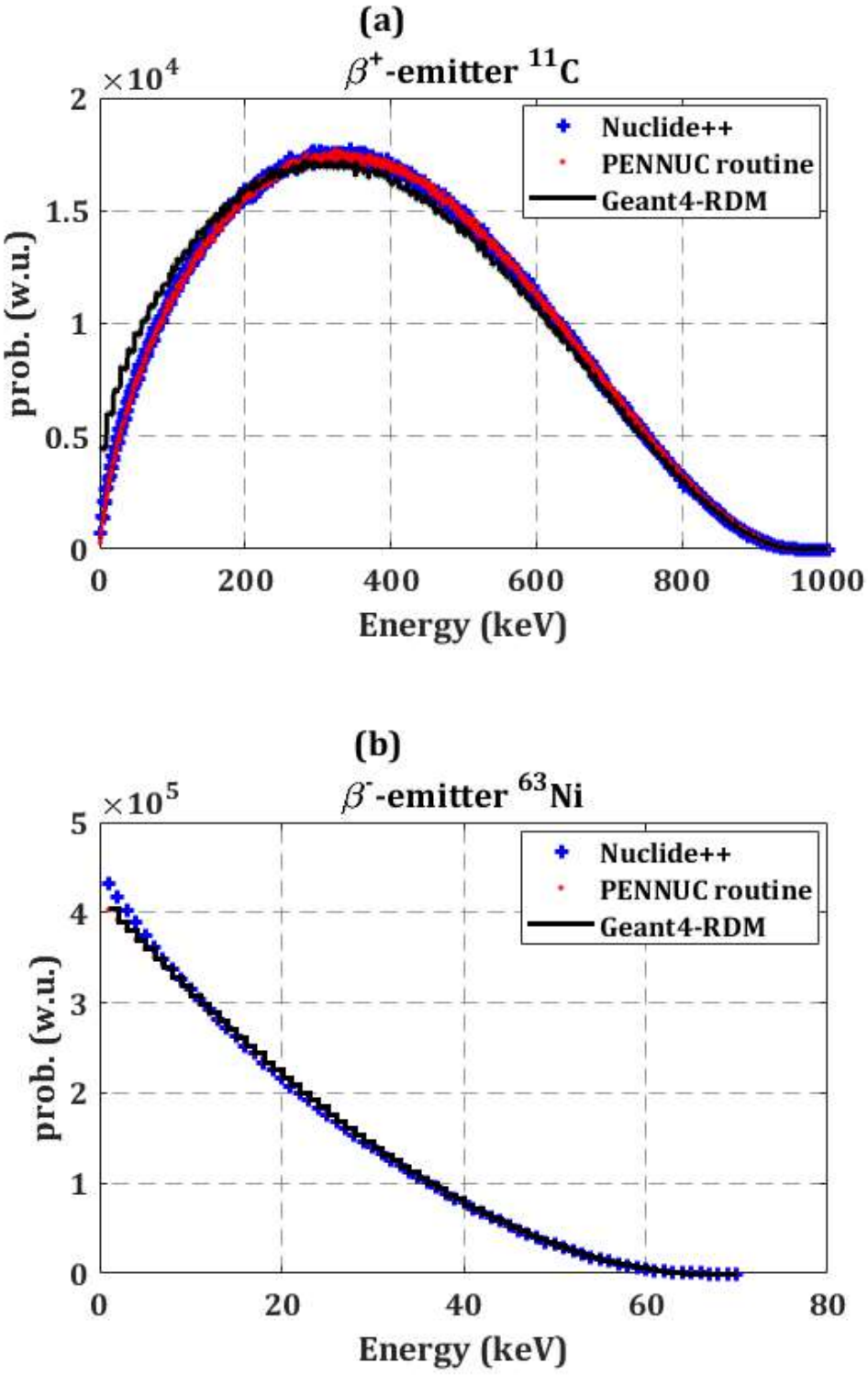
(a)
β^+-emitter ^{11}C
×10^4
2
1.5
1
0.5
0
prob. (w.u.)
0
200
400
600
800
1000
Energy (keV)
Nuclide++
PENNUC routine
Geant4-RDM
(b)
β^--emitter ^{63}Ni
×10^5
5
4
3
2
1
0
prob. (w.u.)
0
20
40
60
80
Energy (keV)
Nuclide++
PENNUC routine
Geant4-RDM

Table 1.

^{152}Eu emissions γ and X-ray	Energy (keV)	Intensity (%)				
		Nuclide++	PENNUC	z-score	G4-RDM	z-score
$X_{K\alpha1}$ (Sm)	40.12	38.26 (6)	38.21 (6)	0.29	38.23 (6)	0.18
$\gamma_{1,0}$ (Sm)	121.78	28.45 (5)	28.46 (5)	0.07	28.33 (5)	0.85
$\gamma_{1,0}$ (Gd)	344.28	26.58 (5)	26.53 (5)	0.35	26.56 (5)	0.14
$X_{K\alpha2}$ (Sm)	39.52	21.164 (46)	21.163 (46)	0.01	21.146 (46)	0.14
$\gamma_{13,1}$ (Sm)	1408.01	20.875 (46)	20.911 (46)	0.28	20.800 (46)	0.58
$\gamma_{9,1}$ (Sm)	964.08	14.390 (38)	14.398 (38)	0.07	14.354 (38)	0.33
$\gamma_{10,1}$ (Sm)	1112.08	13.396 (37)	13.421 (37)	0.24	13.403 (37)	0.07
$\gamma_{7,1}$ (Gd)	778.90	12.948 (36)	12.933 (36)	0.15	12.946 (36)	0.02
$\gamma_{9,0}$ (Sm)	1085.84	10.048 (32)	10.099 (32)	0.56	10.112 (32)	0.71
$\gamma_{2,1}$ (Sm)	244.70	7.566 (28)	7.559 (27)	0.09	7.578 (27)	0.15
$X_{K\beta1}$(Sm)	45.41	7.382 (27)	7.429 (27)	0.62	7.433 (27)	0.67
$X_{L\alpha}$(Sm)	5.64	5.752 (24)	5.792 (24)	0.59	5.800 (24)	0.71
$\gamma_{10,2}$ (Sm)	867.38	4.230 (21)	4.235 (21)	0.08	4.256 (21)	0.44
$X_{K\beta3}$(Sm)	45.29	3.845 (19)	3.867 (20)	0.40	3.820 (20)	0.45
$X_{L\alpha}$ (Sm)	6.20	3.449 (19)	3.640 (19)	3.55	3.630 (19)	3.37
$\gamma_{13,9}$ (Sm)	443.97	3.175 (18)	3.111 (18)	1.26	3.134 (18)	0.81
$\gamma_{3,1}$ (Gd)	411.12	2.228 (15)	2.213 (15)	0.35	2.268 (15)	0.94
$\gamma_{11,1}$ (Gd)	1089.74	1.737 (13)	1.711 (13)	0.71	1.736 (13)	0.03
$\gamma_{14,1}$ (Gd)	1299.14	1.626 (13)	1.612 (13)	0.38	1.627 (13)	0.03
$X_{K\beta2}$ (Sm)	46.63	1.620 (13)	1.586 (13)	0.92	1.626 (13)	0.16
$\gamma_{14,2}$ (Sm)	1212.95	1.421 (12)	1.408 (12)	0.38	1.427 (12)	0.18
$X_{L\alpha}$ (Sm)	6.57	0.962 (10)	1.079 (10)	4.14	1.096 (10)	4.74
$X_{L\alpha}$ (Sm)	6.32	0.749 (9)	0.762 (9)	0.07	0.870 (9)	0.67
$\gamma_{12,2}$ (Sm)	1005.27	0.661 (8)	0.668 (8)	0.04	0.652 (8)	0.06

Table 2.

^{133}Ba **emissions γ and X-ray**	**Energy (keV)**	**Intensity (%)**				
		Nuclide++	**PENNUC**	**z-score**	**G4-RDM**	**z-score**
$X_{KO2,3}$ (Cs)	30.97	63.44 (8)	63.49 (8)	0.22	32.63 (16)	188.82
$\gamma_{4,1}$ (Cs)	356.01	61.51 (8)	61.58 (8)	0.31	61.61 (8)	0.44
$X_{K\alpha 2}$ (Cs)	30.63	34.36 (6)	34.27 (6)	0.53	17.68 (12)	136.30
$\gamma_{1,0}$ (Cs)	80.99	33.27 (6)	33.29 (6)	0.12	33.27 (6)	0.00
$\gamma_{3,1}$ (Cs)	302.85	18.188 (43)	18.161 (43)	0.22	18.294 (43)	0.87
$X_{K\beta 1}$ (Sm)	34.99	11.646 (34)	11.677 (34)	0.32	9.066 (68)	16.97
$\gamma_{3,0}$ (Cs)	383.85	8.908 (30)	8.885 (30)	0.27	9.016 (90)	0.57
$\gamma_{4,2}$ (Cs)	276.40	7.038 (27)	7.074 (27)	0.47	7.130 (37)	1.00
X_L (Cs)	4.29	6.634 (26)	6.698 (26)	0.87	2.748 (52)	33.42
$X_{K\beta 3}$ (Cs)	34.92	6.039 (25)	6.032 (25)	0.10	5.973 (50)	0.59
X_L (Cs)	4.62	3.961 (20)	3.916 (20)	0.80	1.635 (40)	26.01
$\gamma_{2,1}$ (Cs)	79.61	2.666 (16)	2.673 (16)	0.15	2.660 (16)	0.13
$X_{K\beta 2}$ (Cs)	35.82	2.466 (16)	2.468 (15)	0.05	1.924 (38)	6.57
$\gamma_{4,3}$ (Cs)	53.16	2.148 (15)	2.112 (15)	0.85	2.167 (15)	0.45
X_L (Cs)	4.92	1.020 (10)	1.123 (11)	3.46	0.590 (33)	6.24

Table 3.

β-emitting radionuclides	Generated spectrum energy (keV)				
	Nuclide++	**PENNUC**	**Relative difference with Nuclide++**	**Geant4-RDM**	**Relative difference with Nuclide++**
^{11}C	max: 960.0 avg: 384.0	max: 958.2 avg: 386.1	0.2% 0.5%	max: 959.9 avg: 372.5	< 0.1% 3.0%
^{18}F	max: 631.9 avg: 249.5	max: 631.7 avg: 250.4	< 0.1% 0.3%	max: 633.8 avg: 231.0	0.3% 7.4%
^{44}Sc	max: 1472.0 avg: 630.4	max:1472.0 avg: 633.5	0% 0.5%	max: 1472.0 avg: 582.0	0% 7.6%
^{63}Ni	max: 60.0 avg: 17.5	max: 60.0 avg: 17.4	0% 0.6%	max: 60.0 avg: 17.4	0% 0.6%
^{32}P	max: 1709.2 avg: 693.5	max: 1705.5 avg: 694.4	0.2% 0.1%	max: 1709.6 avg: 695.1	< 0.1% 0.2%
^{90}Y	max: 2275.0 avg: 930.5	max: 2272.2 avg: 942.5	0.1% 1.3%	max: 2276.5 avg: 935.4	< 0.1% 0.5%