

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

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OUTLINE

- General introduction
- Brief description of the Geant4 code
- Description of the code Nuclide++ (data, implementation...)
- Validation of Nuclide++ through chosen radionuclides examples
- Conclusion and comment

INTRODUCTION (1)

- **Motivation:**

- Monte Carlo (MC) simulation codes: widely used to assess the response of detectors
- **Radioactive decay (RD) play an important role for many experiments**
 - ✓ particle and nuclear physics, medical physics, ionizing radiation metrology...
 - ✓ comprehensive and accurate knowledge of the decay schemes data is crucial
- **In ionizing radiation metrology:** Penelope and Geant4 are common used
- **PENNUC (Fortran): RD routine using DDEP database is available in Penelope (2017)**
 - ✓ developed at CIEMAT, LNHB – *García-Toraño et al. Nucl. Instrum. Meth. B396 (2017)*
- **Geant4: Radioactive Decay Module is available, based on popular ENSDF data library**
 - ✓ original implémentation: *Lei & Truscott, Tech. Rep. Qinetiq (2002)*, Geant4.9.4-p04 version
 - ✓ functional per-decay approach with a few inconsistencies and missing features
 - ✓ e.g., low intensity emissions not taken into account for certain radionuclides, missing in β -decay (sample continuous decay emission), or deexcitation of the daughter atom...

- **Objective of this work:**

- ➔ **Develop of a new C++ module (*Nuclide++*) for precise simulation of radionuclide sources**
 - ✓ based on DDEP recommended data – *Kellett and Bersillon, EPJ Web Conf. 146 (2017)*

INTRODUCTION (2)

- **The new *Nuclide++* radioactive decay module:**

→ Able to generate decay schemes of radionuclides using DDEP recommended data

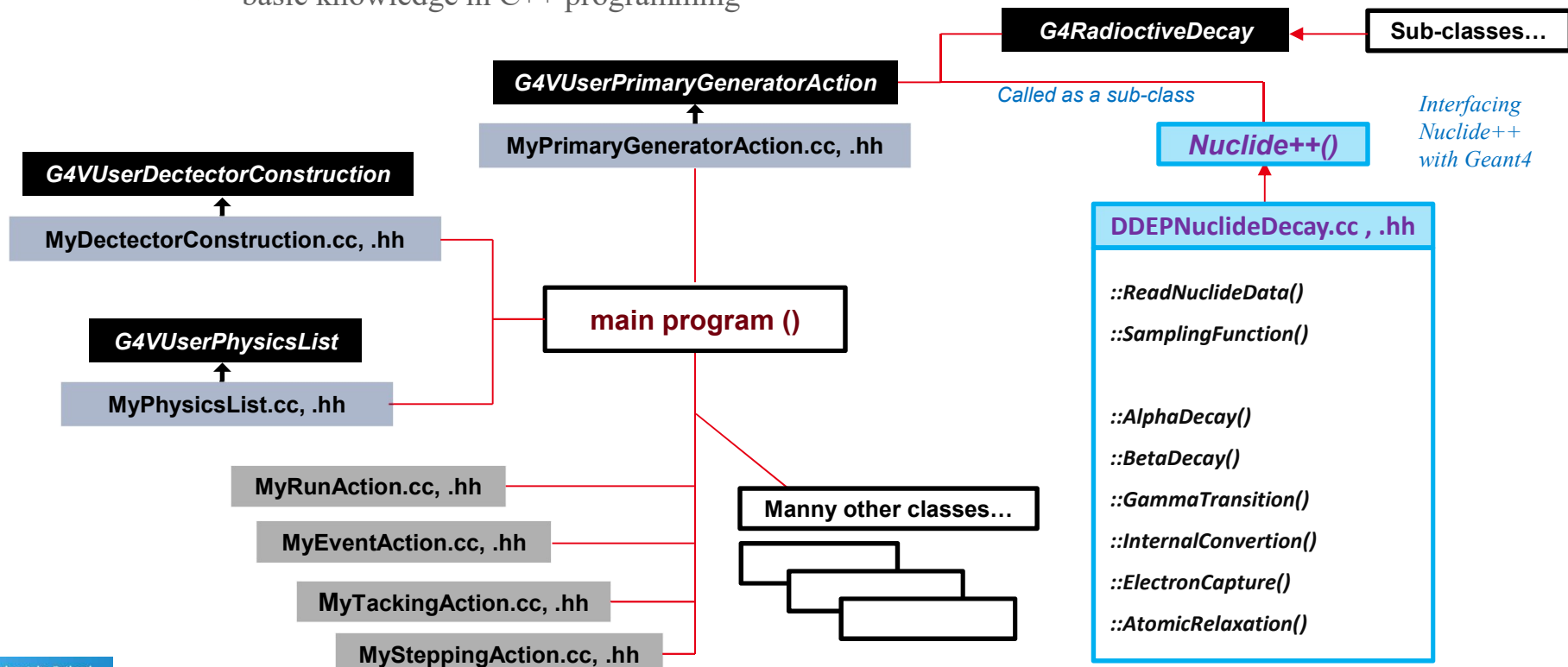
Requirements

- Decay an unstable nucleus
 - sample discrete decay (α , γ) and continuous decay (β^- , β^+) emissions
- Deexcite daughter nucleus
 - sample gamma, X-rays and conversion electrons resulting from atomic deexcitation
 - sample fluorescence and Auger electrons due to shell vacancies
- Simplify the physical process of the radioactive decay and just **generate particles associated to the spontaneous emission of ionizing radiation**
- Improve and detail where necessary
- Handle large number of decays
- Handle decay chains efficiently
- Handle single or multiple radionuclides sources
- **Include time dependence of detectors** (to account for the delay of metastable state)
- **Designed to use transparently in Geant4-based simulation applications**

BRIEF INTRODUCTION TO GEANT4

- **Key Geant4 functionalities**

- General purpose MC simulation tool for the transport of particles through matter
 - ✓ thanks to the polymorphism mechanism of C++, the users can easily plug-in their extensions without interfering with the other part of Geant4
 - ✓ minimal knowledge of the Geant4 structure and base classes
 - ✓ basic knowledge in C++ programming

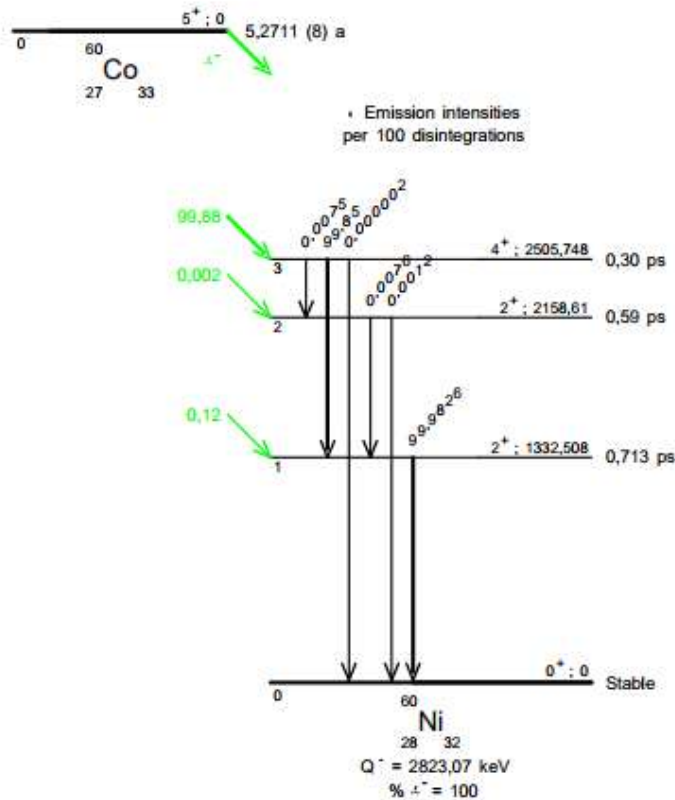


DESCRIPTION OF NUCLIDE++ DATABASE UTILIZED

- The database used consists of the following:
 - (1) **DDEP database exported in specific format**
 - ✓ Contains evaluated and validated atomic and nuclear data published by DDEP (~220 radionuclides)
 - ✓ possible transitions, branching ratios, type/energy of emitted particles → exported in ASCII file
 - (2) **Atom relaxation database: two ASCII files**
 - ✓ **pdatconf.p14**: atomic ground-state configurations, ionization energies, shell details
→ prepared using radiative/non-radiative transition probabilities for sub-shells of elements from LLNL EADL
 - ✓ **pdrelax.p11**: table of transitions, transition probabilities and energies of X-rays/electrons for ionised atoms with a single vacancy in K shell or in an L, M or N subshell
→ from Penelope database
 - ✓ atomic rearrangement sampling on the basis of detailed $KL_1L_2L_3$, M, N, model
– Grau Malonda et al., Comput. Phys. Com. 123 (1999) – Kossert and Grau Carles, Appl. Radiat. Isot. 64 (2006)
 - (3) **BetaShape database**
 - ✓ β spectra generated with **BetaShape** program – Mougéot, Phys. Rev. C91; Phys. Rev. C92 (2015)

DESCRIPTION OF NUCLIDE++ DATABASE UTILIZED

- DDEP exported ASCII data
Co60-PenNuc.txt



```

PAR C060
AZP 60 ; 27
NDA 1
COM ***** Evaluation Date: 13/01/2006 *****
COM ===== Daughter Separator =====
DAU NI60
DDE 1 ; ; 3 ; 3
O 2823.07 ; 0.21
COM ----- Branch Separator -----
BEM 0.9988 ; 0.0003 ; 3 ; 317.32 ; 0.21 ; 0
COM ----- Branch Separator -----
BEM 0.0002 ; ; 2 ; 664.46 ; 0.21 ; -2
COM ----- Branch Separator -----
BEM 0.0012 ; 0.0003 ; 1 ; 1490.56 ; 0.21 ; -2
COM ----- Branch Separator -----
COM ----- Level Separator - T1/2 in seconds -----
LED 2505.748 ; 0.005 ; 9 ; 3.E-13 ; 9.E-14 ; 3
GA 0.000075 ; 0.000004 ; 347.14 ; 0.07 ; 2
EK 0.000000374 ; 0.000000023 ; 338.81 ; 0.07 ; 2
EL 0.0000000377 ; 0.000000023 ; 346.23 ; 0.07 ; 2
GA 0.9985 ; 0.0003 ; 1173.228 ; 0.003 ; 1
EK 0.000151 ; 0.000007 ; 1164.9072 ; 0.003 ; 1
EL 0.00001478 ; 0.0000004 ; 1172.3284 ; 0.003 ; 1
GA 0.00000002 ; 0.000000004 ; 2505.692 ; 0.005 ; 0
EK 0.0000000000156 ; 0.0000000000031 ; 2497.415 ; 0.005 ; 0
EL 0.00000000000152 ; 0.00000000000031 ; 2504.836 ; 0.005 ; 0
COM ----- Level Separator - T1/2 in seconds -----
LED 2158.61 ; 0.03 ; 6 ; 5.9E-13 ; 1.7E-13 ; 2
GA 0.000076 ; 0.000008 ; 826.1 ; 0.03 ; 1
EK 0.0000000228 ; 0.0000000039 ; 817.767 ; 0.03 ; 1
EL 0.00000000221 ; 0.00000000027 ; 825.188 ; 0.03 ; 1
GA 0.000012 ; 0.000002 ; 2158.57 ; 0.03 ; 0
EK 0.00000000053 ; 0.00000000009 ; 2150.277 ; 0.03 ; 0
EL 0.000000000052 ; 0.000000000009 ; 2157.698 ; 0.03 ; 0
COM ----- Level Separator - T1/2 in seconds -----
LED 1332.508 ; 0.004 ; 3 ; 7.13E-13 ; 1.1E-14 ; 1
GA 0.999826 ; 0.000006 ; 1332.492 ; 0.004 ; 0
EK 0.000115 ; 0.000005 ; 1324.1752 ; 0.004 ; 0
EL 0.0000113 ; 0.0000003 ; 1331.5964 ; 0.004 ; 0
    
```



DESCRIPTION OF NUCLIDE++ DATABASE UTILIZED

- Atom relaxation database

Pdatconf.p14

Z	S0	S1	S2	PROBABILITY	ENERGY
3	1	2	0	2.90000E-04	5.43000E+01
3	1	2	2	9.99710E-01	4.80000E+01
4	1	2	0	3.60000E-04	1.08500E+02
4	1	2	2	9.99640E-01	9.64000E+01
5	1	3	0	5.70000E-04	1.83300E+02
5	1	3	3	9.99430E-01	1.69000E+02
6	1	3	0	5.61488E-04	2.77000E+02
6	1	4	0	1.12060E-03	2.77000E+02
6	1	2	2	4.13609E-01	2.55890E+02
6	1	2	3	1.36190E-01	2.64460E+02
6	1	2	4	2.71099E-01	2.64470E+02
6	1	3	3	4.20748E-03	2.73030E+02
6	1	3	4	1.10012E-01	2.73040E+02
6	1	4	4	6.32008E-02	2.73050E+02
7	1	3	0	1.09420E-03	3.92400E+02
7	1	4	0	2.18181E-03	3.92400E+02
7	1	2	2	2.65388E-01	3.58650E+02
7	1	2	3	1.29999E-01	3.70250E+02
7	1	2	4	2.58276E-01	3.70270E+02
7	1	3	3	8.15943E-03	3.81850E+02
7	1	3	4	2.12711E-01	3.81870E+02
7	1	4	4	1.22190E-01	3.81890E+02
8	1	3	0	1.90768E-03	5.24900E+02
8	1	4	0	3.80027E-03	5.24900E+02
8	1	2	2	1.78644E-01	4.78820E+02
8	1	2	3	1.16224E-01	4.93860E+02
8	1	2	4	2.30418E-01	4.93900E+02
8	1	3	3	1.10822E-02	5.08900E+02
8	1	3	4	2.91115E-01	5.08940E+02
8	1	4	4	1.66809E-01	5.08980E+02
9	1	3	0	3.06841E-03	6.76800E+02
9	1	4	0	6.10743E-03	6.76800E+02
9	1	2	2	1.25970E-01	6.16510E+02
9	1	2	3	1.03000E-01	6.35390E+02
9	1	2	4	2.03651E-01	6.35460E+02
9	1	3	3	1.30903E-02	6.54270E+02
9	1	3	4	3.46901E-01	6.54340E+02
9	1	4	4	1.98211E-01	6.54410E+02

Pdatconf.p14

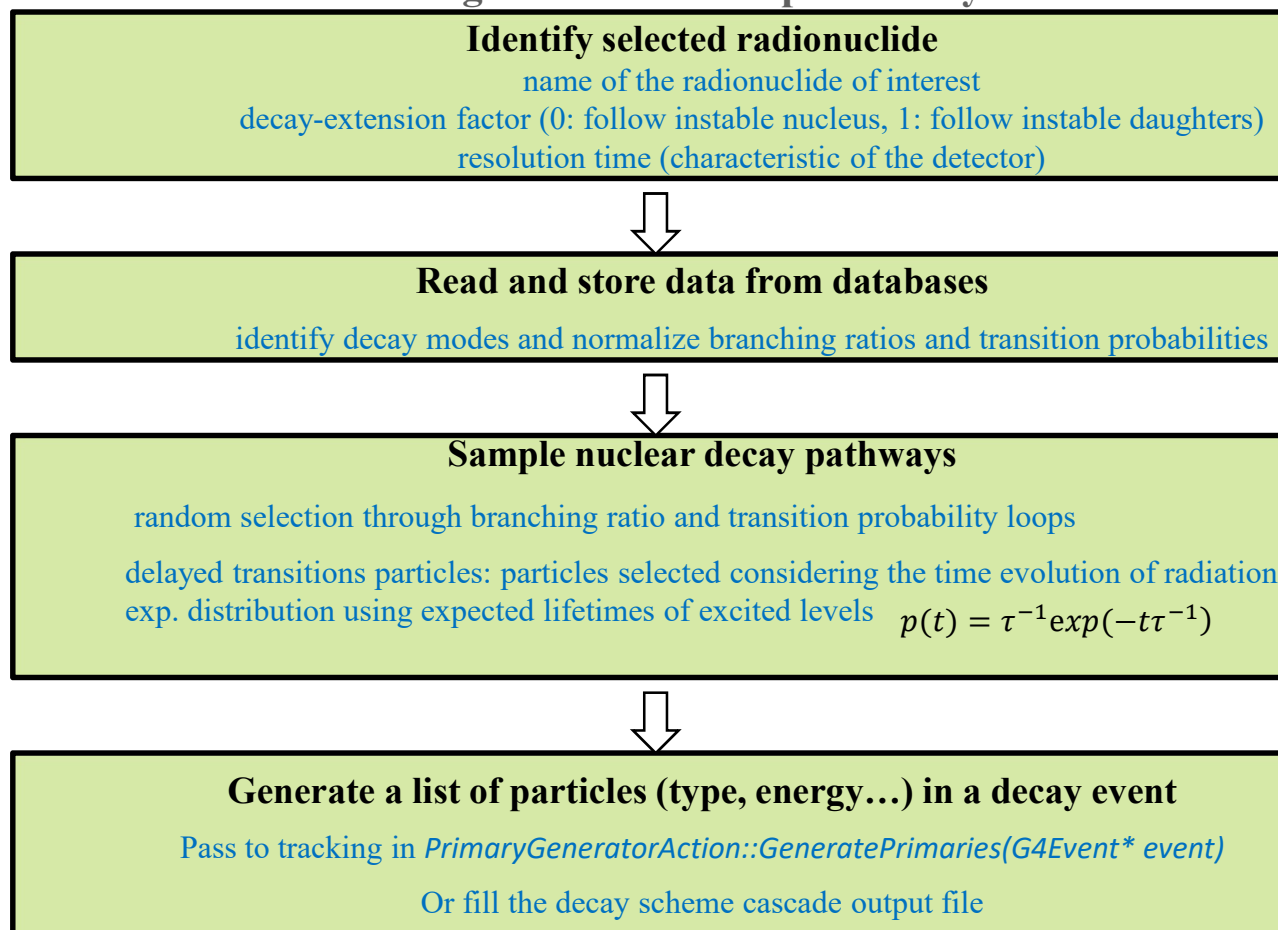
```

# * Ground state configurations, ionization energies, central values
# of Compton profiles, and level widths of free atoms of the elements
# Z=1 to 99.
# ** Ionization energies are from Carlson, 'Photoelectron and Auger
# Spectroscopy' (Plenum Press, New York and London, 1975).
# ** The Compton profiles at P_z=0 were calculated by Salvat from MCDF
# atomic wave functions. These values are more accurate than those of
# Biggs et al. [At. Data and Nucl. Data Tables 16 (1975) 201-309].
# ** Level widths are from the EADL and from Campbell and Papp [At.
# Data and Nucl. Data Tables 77 (2001) 1-56].
#
# +--- Atomic number (Z).
# | +--- Code number of the shell (IS)
# | | +--- Shell (x-ray level notation).
# | | | +--- Shell (spectroscopic notation, nlj).
# | | | | +--- Shell occupation number (f_i).
# | | | | | +--- Ionization energy (eV), in decreasing order.
# | | | | | | +--- One-electron Compton profile at
# | | | | | | | P_z=0 (atomic units).
# | | | | | | | +--- Level widths (eV)
# | | | | | | | | EADL | CampbellPapp
# V V V V V V V V V V
1 1 K 1s1/2 1 1.36000E+01 8.48807E-01 0.00000E+00 0.00000E+00
2 1 K 1s1/2 2 2.45900E+01 5.35207E-01 0.00000E+00 0.00000E+00
3 1 K 1s1/2 2 5.80000E+01 3.28501E-01 0.00000E+00 0.00000E+00
3 2 L1 2s1/2 1 5.39200E+00 1.93549E+00 0.00000E+00 0.00000E+00
4 1 K 1s1/2 2 1.15000E+02 2.36949E-01 0.00000E+00 0.00000E+00
4 2 L1 2s1/2 2 9.32200E+00 1.34238E+00 0.00000E+00 0.00000E+00
5 1 K 1s1/2 2 1.92000E+02 1.85913E-01 0.00000E+00 0.00000E+00
5 2 L1 2s1/2 2 1.13860E+01 1.00114E+00 0.00000E+00 0.00000E+00
5 3 L2 2p1/2 1 1.13860E+01 6.14623E-01 0.00000E+00 0.00000E+00
6 1 K 1s1/2 2 2.88000E+02 1.53080E-01 6.14394E-02 0.00000E+00
6 2 L1 2s1/2 2 1.65900E+01 8.03154E-01 0.00000E+00 0.00000E+00
6 3 L2 2p1/2 2 1.12600E+01 4.88373E-01 0.00000E+00 0.00000E+00
7 1 K 1s1/2 2 4.03000E+02 1.30137E-01 9.27355E-02 0.00000E+00
7 2 L1 2s1/2 2 2.03300E+01 6.71894E-01 0.00000E+00 0.00000E+00
7 3 L2 2p1/2 2 1.45300E+01 4.06903E-01 0.00000E+00 0.00000E+00
7 4 L3 2p3/2 1 1.45300E+01 4.07257E-01 0.00000E+00 0.00000E+00
8 1 K 1s1/2 2 5.38000E+02 1.13183E-01 1.33383E-01 0.00000E+00
8 2 L1 2s1/2 2 2.84800E+01 5.77977E-01 0.00000E+00 0.00000E+00
8 3 L2 2p1/2 2 1.36200E+01 3.49407E-01 0.00000E+00 0.00000E+00
8 4 L3 2p3/2 2 1.36200E+01 3.49884E-01 0.00000E+00 0.00000E+00
9 1 K 1s1/2 2 6.94000E+02 1.00136E-01 1.83627E-01 0.00000E+00
9 2 L1 2s1/2 2 3.78500E+01 5.07272E-01 0.00000E+00 0.00000E+00
9 3 L2 2p1/2 2 1.74200E+01 3.06443E-01 0.00000E+00 0.00000E+00
9 4 L3 2p3/2 3 1.74200E+01 3.07053E-01 0.00000E+00 0.00000E+00
10 1 K 1s1/2 2 8.70100E+02 8.97814E-02 2.42819E-01 2.40000E-01
10 2 L1 2s1/2 2 4.84700E+01 4.52046E-01 0.00000E+00 0.00000E+00
10 3 L2 2p1/2 2 2.16600E+01 2.73020E-01 0.00000E+00 1.00000E-02
10 4 L3 2p3/2 4 2.15600E+01 2.73772E-01 0.00000E+00 1.00000E-02

```


DESCRIPTION OF NUCLIDE++ RADIOACTIVE PROCESS IMPLEMENTED

Flowchart describing the different steps of decays simulation





NUCLIDE++ OUTPUT

```
## =====  
## Nuclide++: a C++ module for radioactive decay  
## Using the DDEP (Decay Data Evaluation Project) recommended data  
## Using BetaShape (Phys. Rev. C91; Phys. Rev. C92) calculated spectra  
## Using atomic relaxation data for each element from pdrelax.pl1 file  
## Using transition probabilities extracted from LLNL (EADL)  
## =====  
## C1 Number of events generated  
## C2 particle energy (eV)  
## C3 particle ID (e-=1, photon=2, positron=3, alpha=4)  
## C4 decay mode ID (IC=11, EC=12, Beta-=13, Beta+=14,  
## Alpha=15, AR=21, Gamma=22)  
## =====  
## =====  
708 344492.700000 1 12  
708 1408013.000000 2 22  
708 121781.700000 2 22  
818 788450.100000 1 12  
818 964079.000000 2 22  
818 121781.700000 2 22  
1372 344492.700000 1 12  
1372 1408013.000000 2 22  
1372 121781.700000 2 22  
1485 344492.700000 1 12  
1485 1408013.000000 2 22  
1485 121781.700000 2 22  
3219 788450.100000 1 12  
3219 964079.000000 2 22  
3219 121781.700000 2 22  
4209 344492.700000 1 12  
4209 1408013.000000 2 22  
4209 121781.700000 2 22  
4375 788450.100000 1 12  
4375 964079.000000 2 22  
4375 121781.700000 2 22  
4475 294935.000000 1 12
```

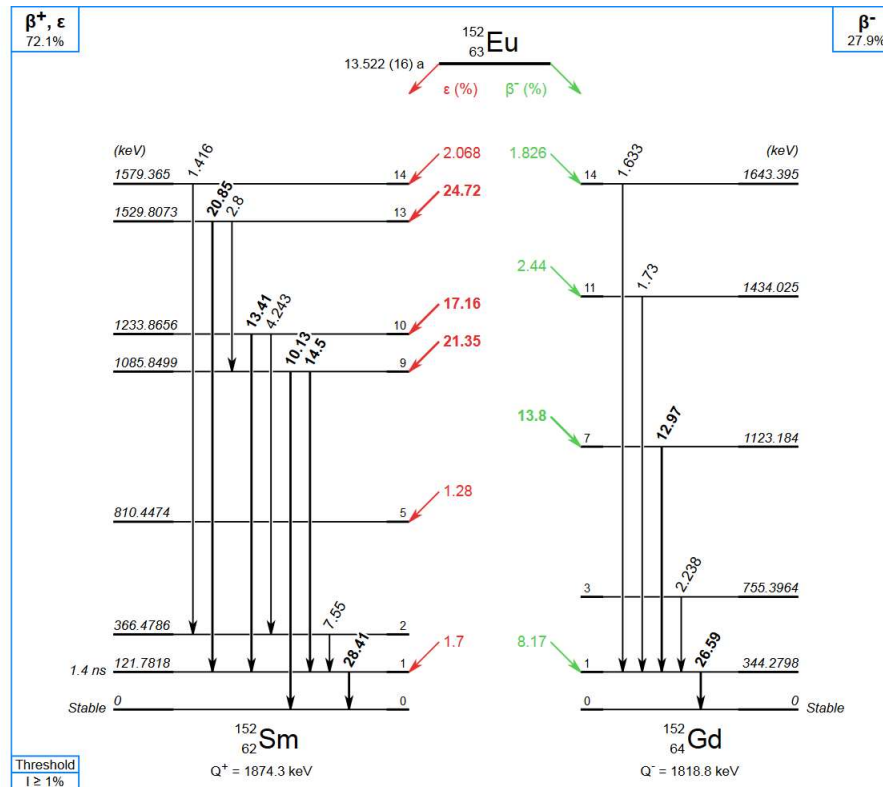
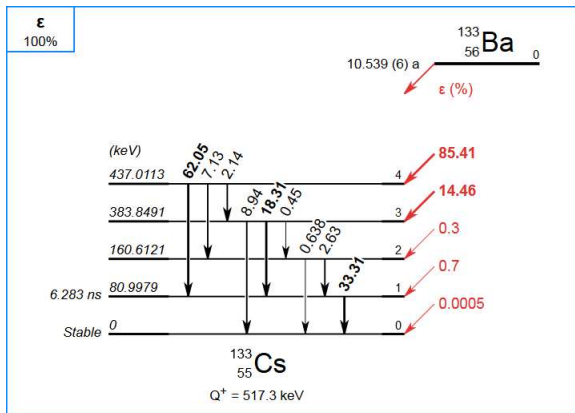
VALIDATION OF NUCLIDE++ MODULE

- **The code implementations verified for consistency with DDEP data**
 - Comparison with PENNUC developed at CIEMAT for Penelope code
 - ✓ well validated and considered in the radionuclide metrology community as a reference
 - comparison against it provides a valuable evaluation
 - Comparison with existing Geant4-RDM
- **Several radionuclide decays tested**
 - γ -emitting radionuclides: ^{152}Eu , ^{133}Ba , ^{60}Co , ^{134}Cs , ^{137}Cs , ^{113}Sn , $^{166\text{m}}\text{Ho}$
 - EC radionuclides: ^{55}Fe , ^{54}Mn , ^{125}I
 - β -emitting radionuclides: ^{11}C , ^{18}F , ^{44}Sc , ^{63}Ni , ^{32}P , ^{90}Y

VALIDATION OF NUCLIDE++ MODULE

¹³³Ba: decays by EC mainly to two ¹³³Cs excited levels of 437 keV (~85.4%) and 384 keV (~14.5%), and with minor branches (<1%) to 161 keV and 81 keV excited levels and to the ground state

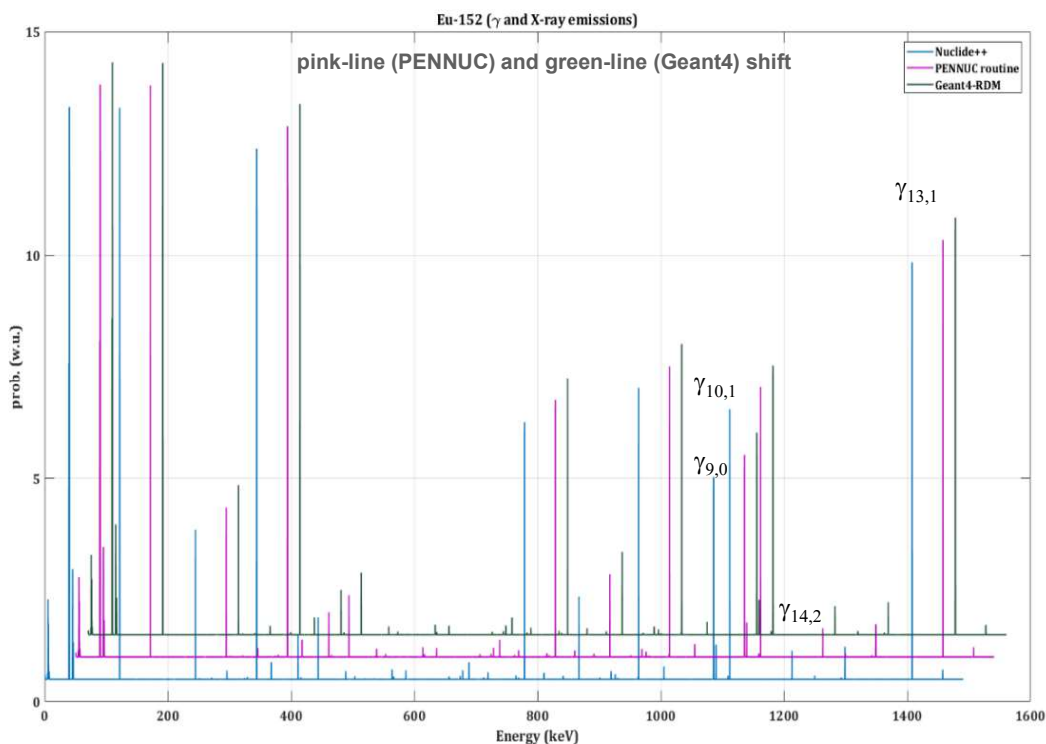
¹⁵²Eu: decays (72.1%) by EC and about 0.027% by emission of positron to ¹⁵²Sm and by beta minus emission (27.9%) to ¹⁵²Gd



VALIDATION OF NUCLIDE++ MODULE

¹⁵²Eu

Comparison of γ and X-ray emissions from ¹⁵²Eu 10⁶ decays, resulting from



Energies and photon intensities of main γ and X-ray emissions from 10⁶ disintegrations of ¹⁵²Eu

¹⁵² Eu emissions γ and X-ray	Energy (keV)	Intensity (%)		
		Nuclide++	PENNUC (Fortran)	G4-RDM
X _{Kα1} (Sm)	40.12	38.26 (6)	38.21 (6)	38.23 (6)
$\gamma_{1,0}$ (Sm)	121.78	28.45 (5)	28.46 (5)	28.33 (5)
$\gamma_{1,0}$ (Gd)	344.28	26.58 (5)	26.43 (5)	26.56 (5)
X _{Kα2} (Sm)	39.52	21.164 (46)	21.163 (46)	21.146 (46)
$\gamma_{13,1}$ (Sm)	1408.01	20.875 (46)	20.911 (46)	20.800 (46)
$\gamma_{9,1}$ (Sm)	964.08	14.390 (38)	14.398 (38)	14.354 (38)
$\gamma_{10,1}$ (Sm)	1112.08	13.396 (37)	13.421 (37)	13.403 (37)
$\gamma_{7,1}$ (Gd)	778.90	12.948 (36)	12.933 (36)	12.946 (36)
$\gamma_{9,0}$ (Sm)	1085.84	10.048 (32)	10.099 (32)	10.112 (32)
$\gamma_{2,1}$ (Sm)	244.70	7.566 (28)	7.559 (27)	7.578 (27)
X _{Kβ1} (Sm)	45.41	7.382 (27)	7.429 (27)	7.433 (27)
X _{Lα} (Sm)	5.64	5.752 (24)	5.792 (24)	5.800 (24)
$\gamma_{10,2}$ (Sm)	867.38	4.230 (21)	4.235 (21)	4.256 (21)
X _{Kβ3} (Sm)	45.29	3.845 (19)	3.867 (20)	3.820 (20)
X _{Lα} (Sm)	6.20	3.449 (19)	3.640 (19)	3.630 (19)
$\gamma_{13,9}$ (Sm)	443.97	3.175 (18)	3.111 (18)	3.134 (18)
$\gamma_{3,1}$ (Gd)	411.12	2.228 (15)	2.213 (15)	2.268 (15)
$\gamma_{11,1}$ (Gd)	1089.74	1.737 (13)	1.711 (13)	1.736 (13)
$\gamma_{14,1}$ (Gd)	1299.14	1.626 (13)	1.612 (13)	1.627 (13)
X _{Kβ2} (Sm)	46.63	1.620 (13)	1.586 (13)	1.626 (13)
$\gamma_{14,2}$ (Sm)	1212.95	1.421 (12)	1.408 (12)	1.427 (12)
X _{Lα} (Sm)	6.57	0.962 (10)	1.079 (10)	1.096 (10)
X _{Lα} (Sm)	6.32	0.749 (9)	0.762 (9)	0.870 (9)
$\gamma_{12,2}$ (Sm)	1005.27	0.661 (8)	0.668 (8)	0.652 (8)

VALIDATION OF NUCLIDE++ MODULE

¹³³Ba

Gamma Emissions

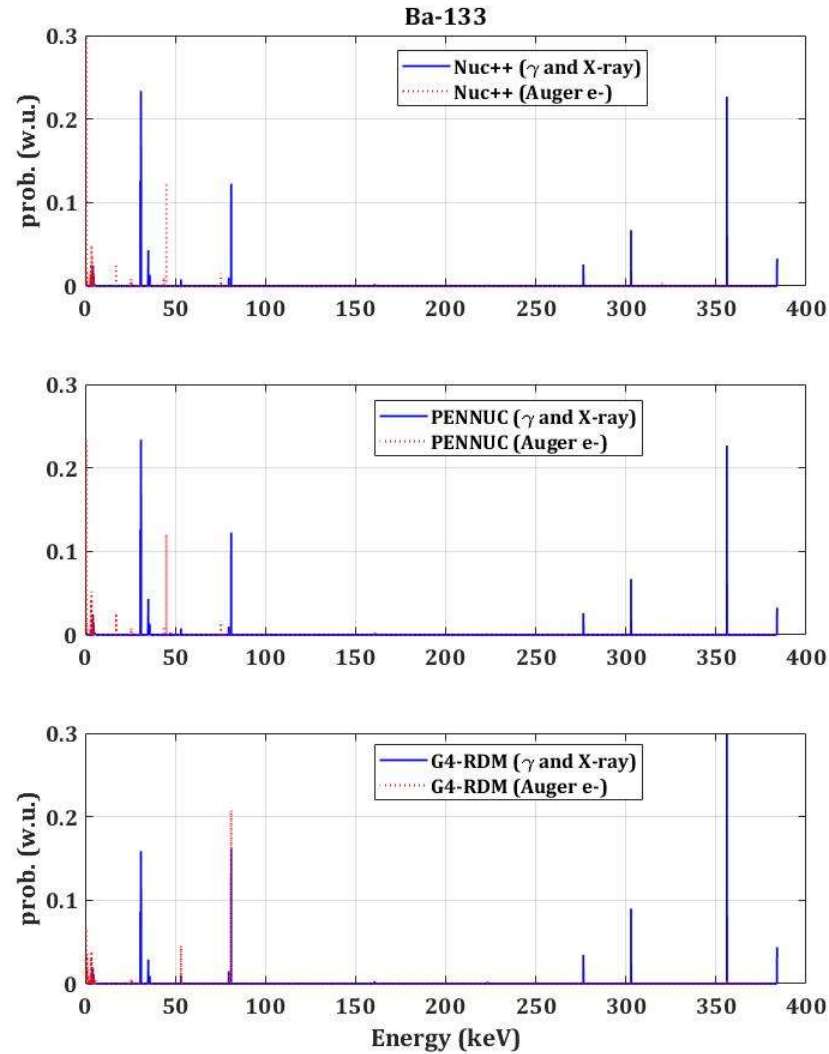
	Energy (keV)	Photons (per 100 disint.)
^{74,3} (Cs)	53,1622 (18)	2,14 (6)
^{72,1} (Cs)	79,6142 (19)	2,63 (19)
^{71,0} (Cs)	80,9979 (11)	33,31 (30)
^{72,0} (Cs)	160,6121 (16)	0,638 (6)
^{73,2} (Cs)	223,2368 (13)	0,450 (5)
^{74,2} (Cs)	276,3989 (12)	7,13 (6)
^{73,1} (Cs)	302,8508 (5)	18,31 (11)
^{74,1} (Cs)	356,0129 (7)	62,05 (19)
^{73,0} (Cs)	383,8485 (12)	8,94 (6)

X-Ray Emissions

	Energy (keV)	Photons (per 100 disint.)	
XL (Cs)	3,7946 - 5,5525	15,87 (26)	
XK _{α2} (Cs)	30,6254	33,8 (4)	} K _α
XK _{α1} (Cs)	30,9731	62,4 (7)	
XK _{β2} (Cs)	34,9197	} 18,24 (29)	} K' β ₁
XK _{β1} (Cs)	34,9873		
XK _{β5'} (Cs)	35,252		
XK _{β2} (Cs)	35,822	} 4,45 (12)	} K' β ₂
XK _{β1} (Cs)	35,907		
XK _{O2,3} (Cs)	35,972		

Auger Electrons

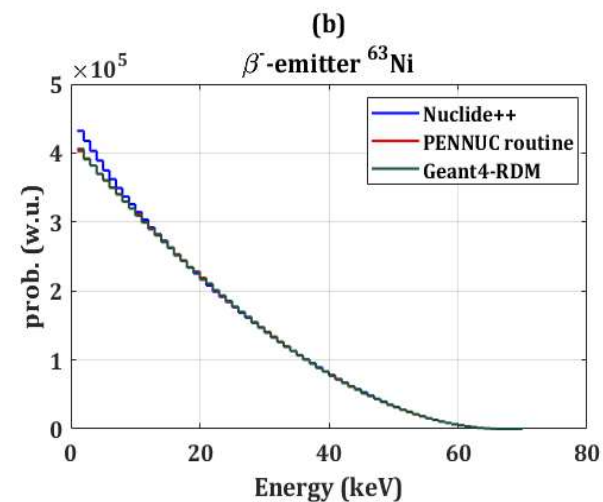
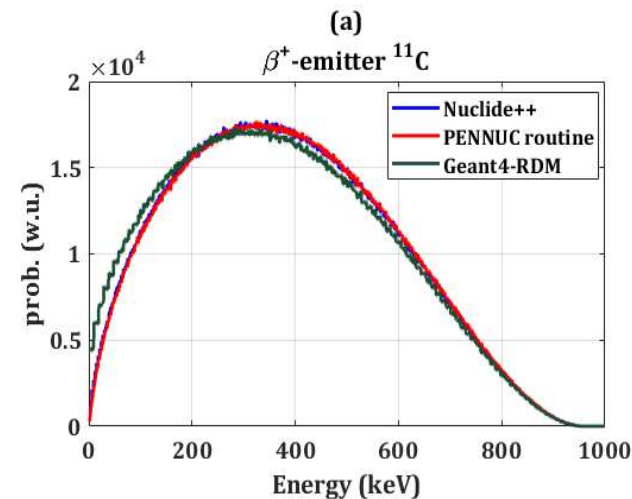
	Energy (keV)	Relative probability
Auger K		
KLL	24,411 - 25,804	100
KLX	28,991 - 30,961	47,2
KXY	33,55 - 35,96	5,56
Auger L	2,5777 - 5,5590	



VALIDATION OF NUCLIDE++ MODULE

β -emitting radionuclides

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



CONCLUSION AND COMMENT

- **NUCLIDE++:** developed to improve the simulation of radioactive sources, offer an alternative to the existing RDM in Geant4
 - ✓ Takes advantage of **DDEP recommended data** for metrological applications
 - ✓ Takes advantage of **BetaShape program**, for improving the nuclear data related to β emission properties
 - ✓ **Good agreement with the Fortran PENNUC subroutine (electron/photons)**
 - ✓ Comparing to Geant4-RDM, α and γ -emission intensities are consistent
 - ✓ **Significant consistency improvements are obtained especially for β -emitting radionuclides**, and atomic rearrangement induced by EC or IC
 - ✓ Ready to use in Geant4-based simulation applications
 - ✓ **The outcome cascade file can be used independently for other applications**
 - ➔ Discrete emitted spectrum can be use to test algorithms in nuclear instrumentation
 - ✓ Advanced test must be performed for the simulation of mixed sources (efficient generation of a large number of decays, time and memory consuming...)
 - ✓ Propagation of uncertainties associated to the decay scheme data
- **In the future, the module will be proposed on the LNHB website**

THANK YOU FOR YOUR ATTENTION !

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