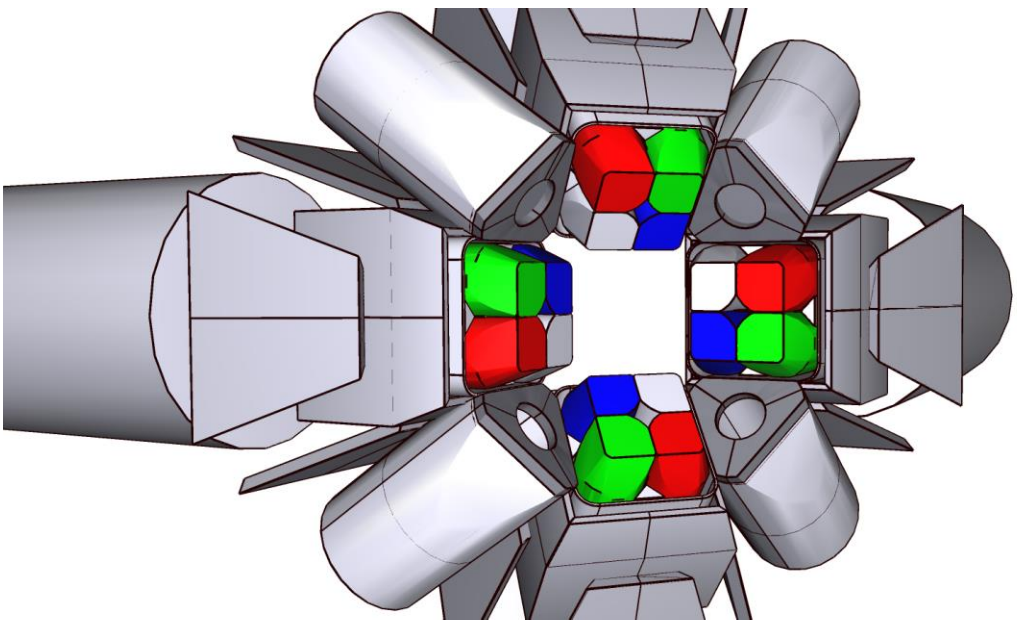
THE UNIVERSITY OF GUELPH

Geant4 Gamma-Gamma Angular Correlations

Geant4 Version 10



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This document outlines the capabilities and operation of the gamma-gamma angular correlations code in Geant4. The code responsible for the gamma-gamma angular correlations was written as an extension to the existing radioactive decay module in Geant4.10.

The radioactive decay module is available in the latest versions of Geant4. There are many good resources online that describe the use of the radioactive decay module, here are a few:

Radioactive Decays in Geant4

Validation of Geant4-based Radioactive Decay Simulation

SLAC Geant4 Tutorial 2014 (See “Hadronic Physics III” presentation)

The simulations outlined in this document were run on the Geant4 virtual machine provided by the IN2P3 group [1]. The gamma-gamma angular correlations code has been tested on the most recent patch (patch 02) of Geant4 version 10.

Outline

1. Introduction to the Radioactive Decay Module

The radioactive decay module is incredibly powerful, and has many benefits over a user-defined decay class implemented in the PrimaryGeneratorAction class. Firstly, the radioactive decay code is maintained, tested and validated by the Geant4 collaboration. The benefit of this should be obvious. Secondly, there are nearly 3000 nuclides with predefined decay files. These decay files, which contain the level structure, branching ratios, gamma-ray energies, internal conversion coefficients, etc, are derived directly from Evaluated Nuclear Structure Data Files (ENSDF). Lastly, there are many integrated features that would be difficult for the user to implement directly into a PrimaryGeneratorAction class.

- Decays in flight or at rest
- Chain of decays towards stability
- Atomic relaxation (x-ray fluorescence, Auger electrons, etc.)
- Calculation of forbidden beta decay spectrum shapes
- Biased sampling of specific decay modes

Here are a couple quick examples on how to run the radioactive decay package. These examples were simulated using version 10 of the GRIFFIN Geant4 simulation code. To utilize Geant4's radioactive decay module the radioactive decay physics must be included in the PhyslicsList class (G4RadioactiveDecayPhysics.hh) of the simulation.

The first example illustrates using the radioactive and photon evaporation files directly. In the next example we copy the files and edit them to our specific needs.

Example 1

The user can use the radioactive and photon evaporation files directly, without ever touching or seeing the input files. Here is an extremely simple example using a source of ^{60}Co. Figure 1 shows the input run macro for this simple decay. The first line loads the particle gun with an ion. The next line tells the simulation the ion is ^{60}Co (in its ground state). Finally the last line tells the simulation to "fire" this ion one million times. No position, direction, or gamma-ray multipolarity information was given so these ions will be positioned at the origin and decay isotropically.

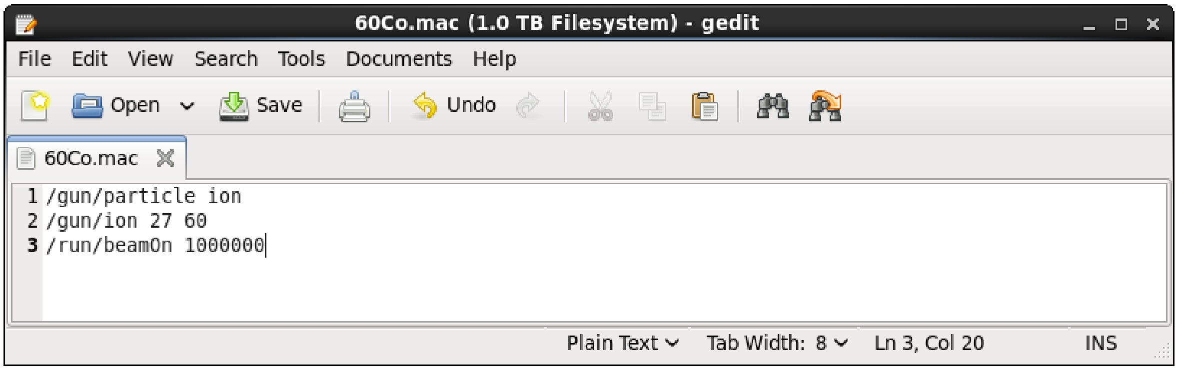


Figure 1 - Run macro for ^{60}Co decay.

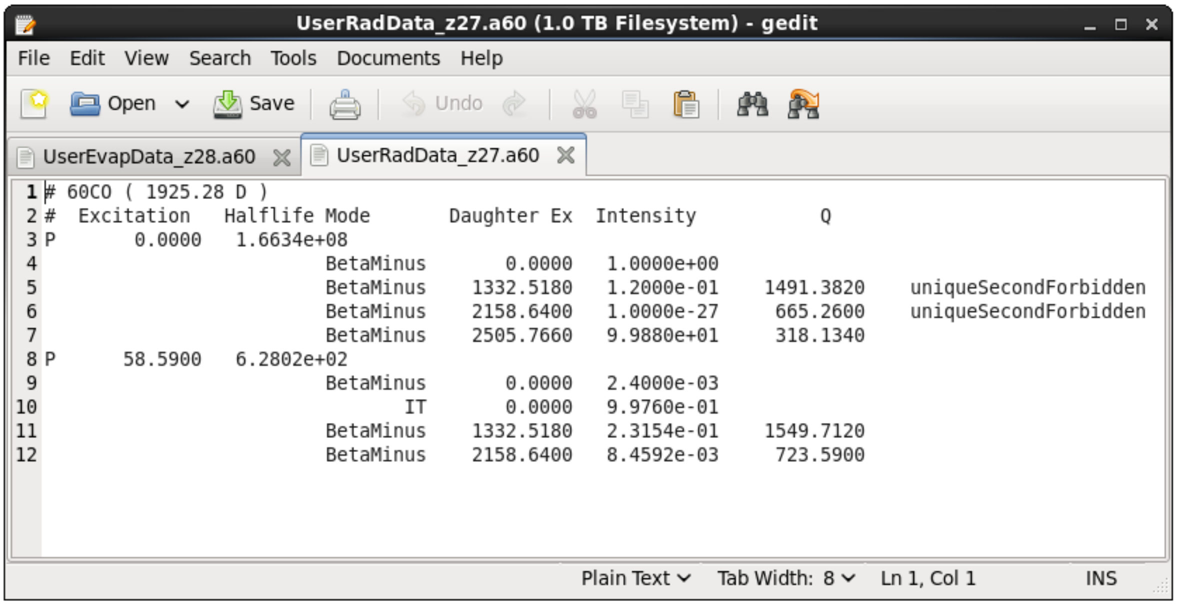
Example 2

Now we would like to see exactly what decay we are simulating. Let's make a new directory in our simulation directory named "UserData", this is where we will store our modified input files.

The first file we need is the ^{60}Co radioactive decay file. In my installation of Geant4 these data files were found in the following directory:

`/usr/local/geant4.10.00/share/Geant4-10.0.0/data/RadioactiveDecay4.0/`

Copy the "z27.a60" file into our "UserData" directory and rename this file to "UserRadData_z27.a60". This file includes the ^{60}Co decay modes, branching ratios, etc. Figure 2 illustrates the radioactive decay input file for ^{60}Co. A complete description of this input file can be found in the file `README_RDM` in the `RadioactiveDecay4.0` directory.



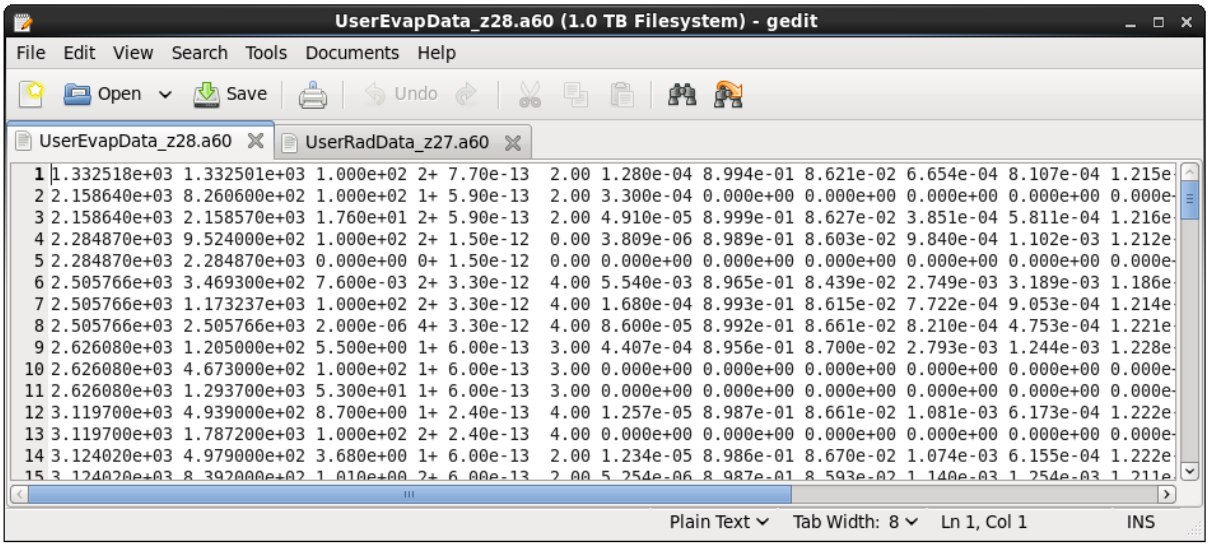

```
# 60CO ( 1925.28 D )
#  Excitation   Halflife Mode       Daughter Ex  Intensity          Q
P      0.0000   1.6634e+08
                         BetaMinus      0.0000   1.0000e+00
                         BetaMinus   1332.5180   1.2000e-01     1491.3820    uniqueSecondForbidden
                         BetaMinus   2158.6400   1.0000e-27      665.2600    uniqueSecondForbidden
                         BetaMinus   2505.7660   9.9880e+01      318.1340
P     58.5900   6.2802e+02
                         BetaMinus      0.0000   2.4000e-03
                                IT      0.0000   9.9760e-01
                         BetaMinus   1332.5180   2.3154e-01     1549.7120
                         BetaMinus   2158.6400   8.4592e-03      723.5900
```

Figure 2 - Radioactive decay file for ^{60}Co.

The next file we need is the photon evaporation file of the daughter nucleus. In my installation of Geant4 these data files were found in the following directory:

`/usr/local/geant4.10.00/share/Geant4-10.0.0/data/PhotonEvaporation3.0/`

Copy the "z28.a60" file into our UserData directory and rename this file to "UserEvapData_z28.a60". This file includes the ^{60}Ni levels, gamma-ray energies, internal conversion coefficients, etc. Figure 3 illustrates the photon evaporation input file for ^{60}Ni. A complete description of this input file can be found in the `README-LevelGammaData` file in the `PhotonEvaporation3.0` directory.

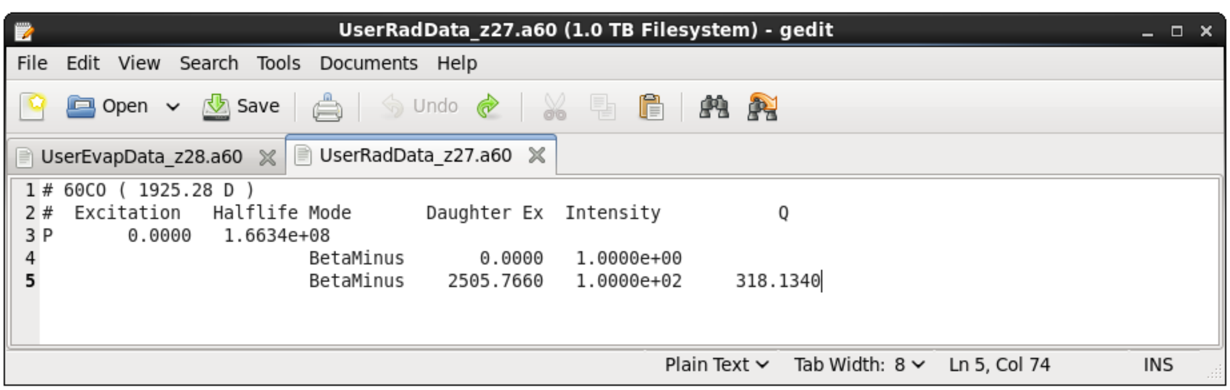


```
1.332518e+03 1.332501e+03 1.000e+02 2+ 7.70e-13  2.00 1.280e-04 8.994e-01 8.621e-02 6.654e-04 8.107e-04 1.215e
2.158640e+03 8.260600e+02 1.000e+02 1+ 5.90e-13  2.00 3.300e-04 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
2.158640e+03 2.158570e+03 1.760e+01 2+ 5.90e-13  2.00 4.910e-05 8.999e-01 8.627e-02 3.851e-04 5.811e-04 1.216e
2.284870e+03 9.524000e+02 1.000e+02 2+ 1.50e-12  0.00 3.809e-06 8.989e-01 8.603e-02 9.840e-04 1.102e-03 1.212e
2.284870e+03 2.284870e+03 0.000e+00 0+ 1.50e-12  0.00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
2.505766e+03 3.469300e+02 7.600e-03 2+ 3.30e-12  4.00 5.540e-03 8.965e-01 8.439e-02 2.749e-03 3.189e-03 1.186e
2.505766e+03 1.173237e+03 1.000e+02 2+ 3.30e-12  4.00 1.680e-04 8.993e-01 8.615e-02 7.722e-04 9.053e-04 1.214e
2.505766e+03 2.505766e+03 2.000e-06 4+ 3.30e-12  4.00 8.600e-05 8.992e-01 8.661e-02 8.210e-04 4.753e-04 1.221e
2.626080e+03 1.205000e+02 5.500e+00 1+ 6.00e-13  3.00 4.407e-04 8.956e-01 8.700e-02 2.793e-03 1.244e-03 1.228e
2.626080e+03 4.673000e+02 1.000e+02 1+ 6.00e-13  3.00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
2.626080e+03 1.293700e+03 5.300e+01 1+ 6.00e-13  3.00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
3.119700e+03 4.939000e+02 8.700e+00 1+ 2.40e-13  4.00 1.257e-05 8.987e-01 8.661e-02 1.081e-03 6.173e-04 1.222e
3.119700e+03 1.787200e+03 1.000e+02 2+ 2.40e-13  4.00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
3.124020e+03 4.979000e+02 3.680e+00 1+ 6.00e-13  2.00 1.234e-05 8.986e-01 8.670e-02 1.074e-03 6.155e-04 1.222e
3.124020e+03 8.392000e+02 1.010e+00 2+ 6.00e-13  2.00 5.254e-06 8.987e-01 8.593e-02 1.140e-03 1.254e-03 1.211e
```

Figure 3 - Photon evaporation file for ^{60}Ni

We can simply change the properties of the decay by modifying these two input files. For example, we can modify the half-life and branching ratios in the radioactive decay input file, and we can add and remove levels and transitions in the daughter nucleus in the photon evaporation input file.

Figures 4 and 5 illustrate modifications to these two input files. In this example modification, all beta decays of ^{60}Co will feed the 2505.8 keV level in ^{60}Ni. And ^{60}Ni will only contain two excited states, 2505.8 keV and 1332.5 keV. The 2505.8 keV level can gamma decay (or internally convert) to the 1332.5 keV level via a 1173.2 keV gamma-ray. And the 1332.5 keV level can gamma decay (or internally convert) to the ground state. We will call this our "simple" ^{60}Co decay.



```
# 60CO ( 1925.28 D )
#  Excitation   Halflife Mode       Daughter Ex  Intensity          Q
P       0.0000   1.6634e+08
                         BetaMinus       0.0000   1.0000e+00
                         BetaMinus    2505.7660   1.0000e+02     318.1340
```

Figure 4 - Modified radioactive decay file for ^{60}Co.

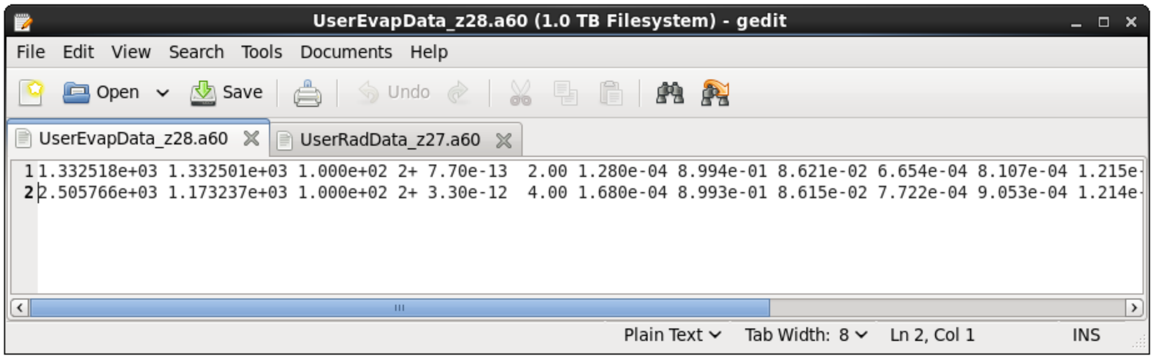


Figure 5 - Modified photon evaporation file for ^{60}Ni

To run our new simple ^{60}Co radioactive decay we need to modify our run macro. Two new macro commands are needed to tell Geant4 we are providing our own input files. The commands are:

```
/grdm/setRadioactiveDecayFile
/grdm/setPhotoEvaporationFile
```

Both commands require 3 inputs. The first input is the Z of the nucleus, the second input is the A of the nucleus, and the last input is the location of the input file. Figure 6 shows our new modified run macro.

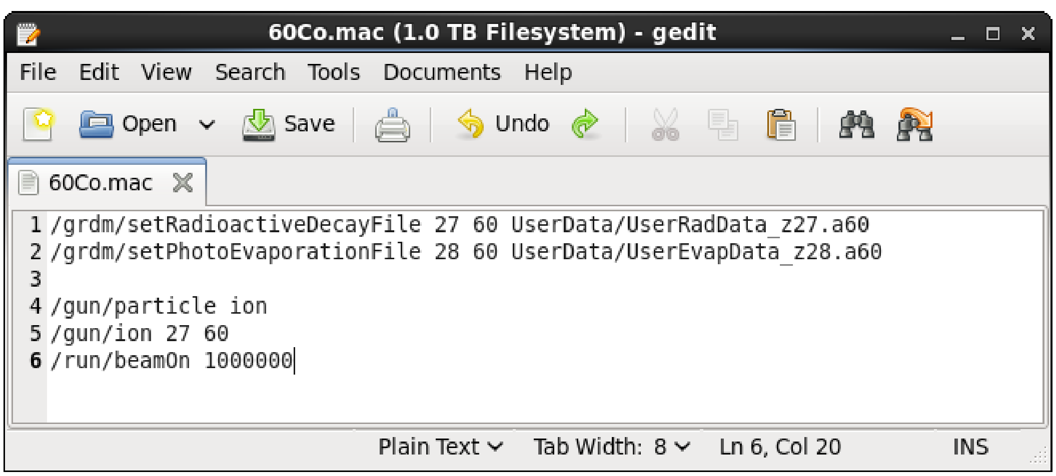


Figure 6 - Run macro for modified ^{60}Co decay.

Now the simulation will decay the ^{60}Co nucleus according to our simple ^{60}Co input files.

2. Installing Gamma-Gamma Correlations Extension

The gamma-gamma correlations code has been appended onto the existing radioactive decay and photon evaportion code, and consequently, includes **no** new classes in the source code of Geant4. The gamma-gamma correlations code has modified two classes in the radioactive decay code and five classes in the photon evaporation code. The two radioactive decay classes are:

```
G4RadioactiveDecay
G4RadioactiveDecaymessenger
```

And the five photon evaporation classes are:

```
G4DiscreteGammaTransition
G4NuclearLevel
G4NuclearLevelManager
G4NuclearLevelStore
G4VGammaDeexcitation
```

To use the gamma-gamma correlations code these new modified classes must overwrite the existing classes in the source directory of Geant4. In my installation of Geant4 these source files can be found in the following directories:

```
/usr/local/src/geant4.10.00/source/processes/hadronic/models/…
radioactive_decay/
/usr/local/src/geant4.10.00/source/processes/hadronic/models/…
de_excitation/photon_evaporation/
```

Once the old Geant4 code is overwritten with the new code we need to rebuild and install Geant4. In my installation of Geant4 the build directory is located here:

```
/usr/local/src/build
```

A simple "make" and "make install" should reinstall Geant4. For help installing Geant4 please refer to the user support webpage.

3. Running Simulations

To run the gamma-gamma correlations code, two additional inputs are required. The first input is the "multipole" file which has a similar format to the photon evaporation file and includes the gamma-ray multipolarity information and mixing ratios. The second input is the ground state angular momentum of the daughter nucleus. If these inputs are not provided, the gamma-rays will be emitted isotropically as intended in the unmodified radioactive decay module.

The photon evaporation file does include a column for the multipolarity of the gamma-ray transition (see `README-LevelGammaData`), but only this one column. There is no option for mixed transitions. We could have modified the photon evaporation input file to include mixed transitions, but that would require the user to modify every photon evaporation file, even if the gamma-gamma correlations code was not being used. Instead, we include another input file for gamma-gamma correlations. The format of this multipole file is described below.

The first two columns are identical to the first two columns of the photon evaporation input file, the first column is the level energy in keV, and the second column is the gamma ray energy in keV. The next two columns describe the multipolarity of the gamma-ray transition, the first column is "L1" and the second column is "L2". The last column is the mixing ratio (δ). For example, if the gamma-ray transition has a pure, unmixed, multipolarity only L1 is needed. In this scenario L2 and delta are set to zero. If the transition is mixed, consider an M1+E2 transition, then L1 is set to 1 and L2 is set to 2 and delta describes the mixing by,

$$\delta = \frac{<L2>}{<L1>}.$$

The second required input is the angular momentum of the nucleus ground state. The radioactive decay and photon evaporation input files do not provide ground state information, only excited states. Therefore, to properly describe the full correlated decay to the ground state, the angular momentum of the ground state is needed.

Example 3 illustrates the use of these input files.

Example 3

In Example 2 we generated two input files for a “simple” ^{60}Co decay, see Figures 4 and 5. We will add gamma-ray multipolarity information to this simple simulation. In the UserData directory we will need to create a multipole file, let’s name it

"UserMultipoleData_z28.a60". The 1173.2 keV and 1332.5 keV gamma-rays are both pure E2 transitions, as shown in the input file in Figure 7.

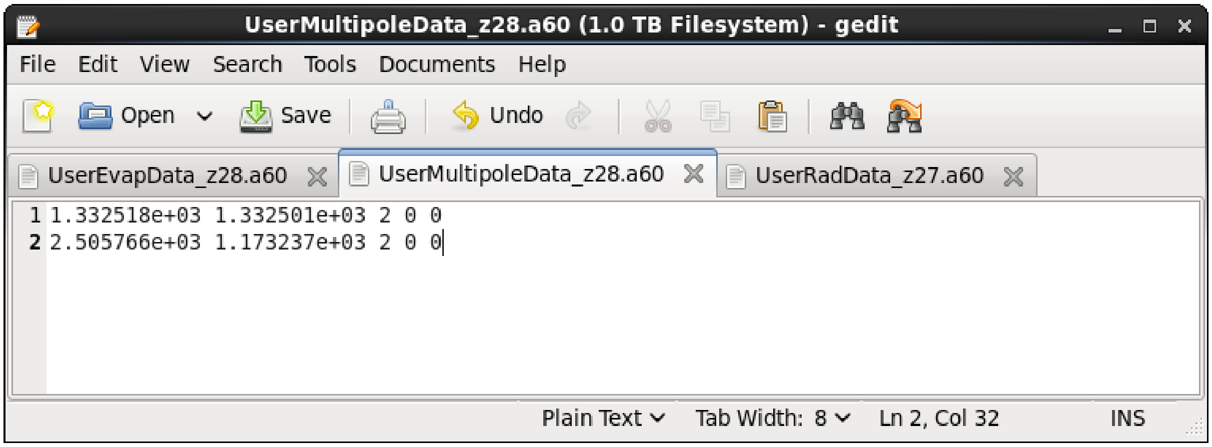


Figure 7 - Multipolarity file for ^{60}Ni.

Now we need to modify the run macro and add the following two commands:

```
/grdm/setMultipoleFile
/grdm/setMultipoleGroundStateSpinAngularMomentum
```

The first command requires three inputs, the Z of the nucleus, the A of the nucleus, and the location of the gamma-ray multipolarity input file. The second command also requires three inputs, the Z of the nucleus, the A of the nucleus, and the angular momentum of the ground state. Figure 8 illustrates the format of the new run macro.

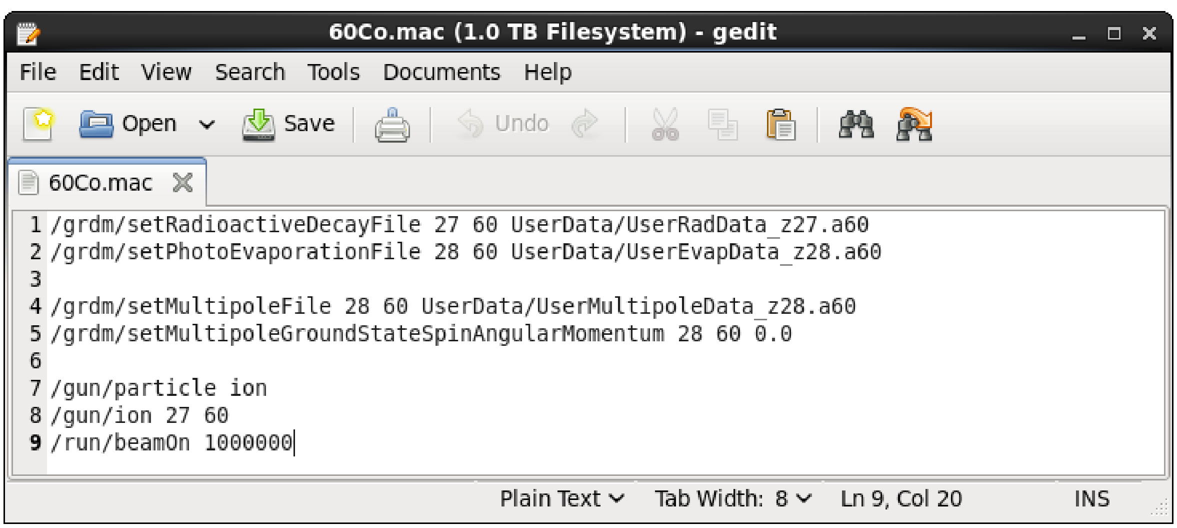


Figure 8 - Run macro providing gamma-ray multipolarity information for ^{60}Co decay.

The result of one million decays of this simple ^{60}Co simulation is shown in Figure 9. In this simulation the 2505.8 keV level is a 4^+, the 1332.5 keV level is a 2^+ and the ground is a 0^+. All gamma-ray transitions are pure E2 transitions. For this decay we expected the correlation coefficients a_2 and a_4 to be 0.1020 and 0.0091 respectively. Our fit, shown in Figure 9, does reasonably well reproducing these correlation coefficients given the number of statistics.

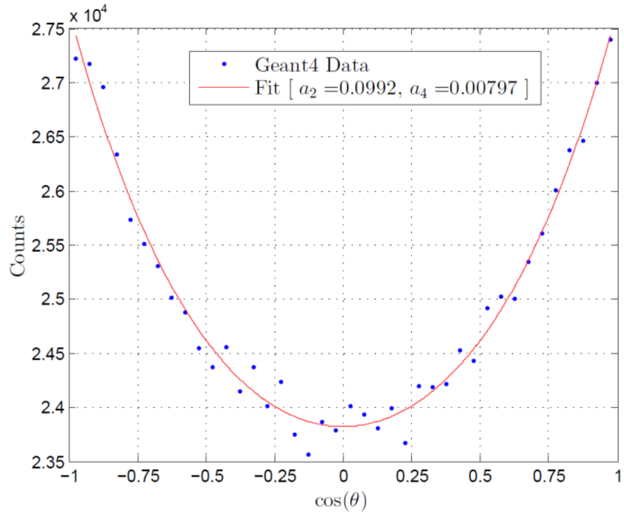


Figure 9 - Correlation of the two gamma-rays in the simple ^{60}Co decay.

Example 4

In this example, for demonstration purposes only, we make a completely unrealistic decay of ^{60}Co. Figure 10 illustrates the simulated decay scheme. The angular momentum of each level was chosen to generate a strong correlation between the pairs of gamma-ray transitions. Figure 11 shows the results of one million decays of this simulation. We expect the correlation coefficients to be a_2 = 0.3571 and a_4 = 1.1429 for the 0^+ - 2^+ - 0^+ cascade, and a_2 = -0.0765 and a_4 = 0.3265 for the 2^+ - 2^+ - 0^+ cascade. Our fit from the simulation results do a very good job reproducing these correlation coefficients.

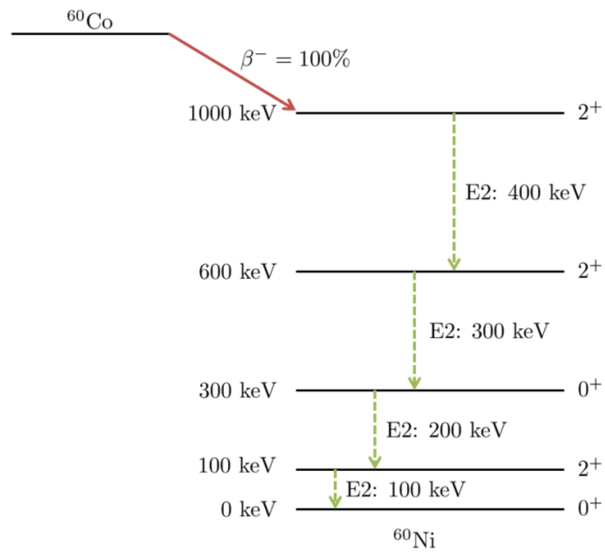


Figure 10 - Unrealistic decay scheme of ^{60}Co.

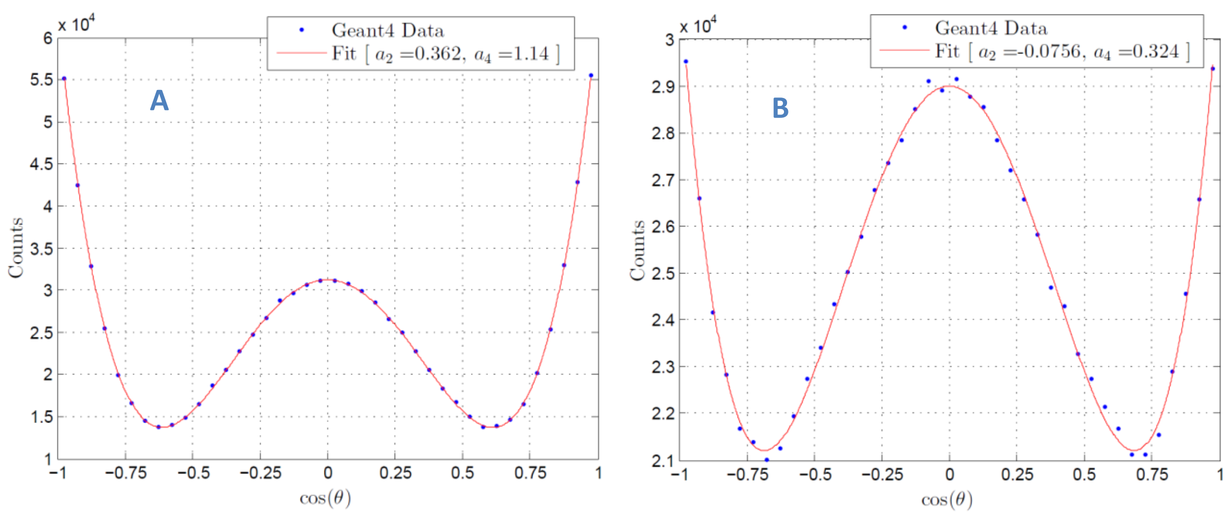


Figure 11 – Simulation and fit results of the correlation of the: [A] 100 and 200 keV gamma-rays. [B] 300 and 400 keV gamma-rays.

Example 5

In this example we make another completely unrealistic decay of ^{60}Co. Figure 12 illustrates the simulated decay scheme. In this decay scheme we have added a mixed M1+E2 transition and two pure M1 transitions. Figure 13 shows the results of one million decays of this simulation. We expect the correlation coefficients to be $a_2 = 0.5$ and $a_4 = 0.0$ for the 0^+ - 1^+ - 0^+ cascade, and $a_2 = 0.4527$ and $a_4 = 0.1633$ for the mixed 2^+ - 2^+ - 0^+ cascade. Our fit from the simulation results do a very good job reproducing these correlation coefficients.

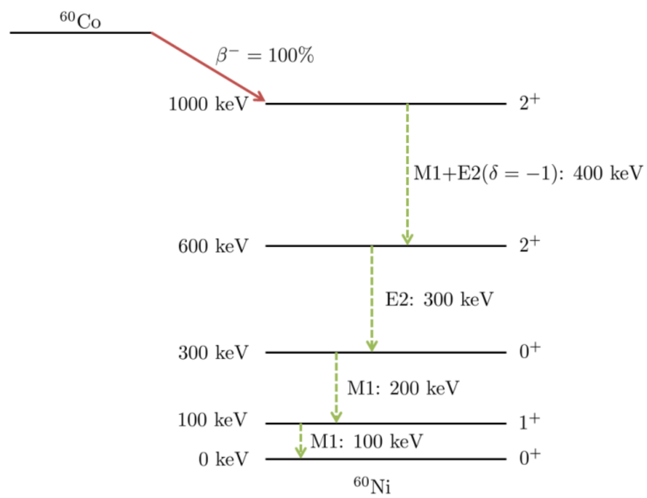


Figure 12- Unrealistic decay scheme of ^{60}Co.

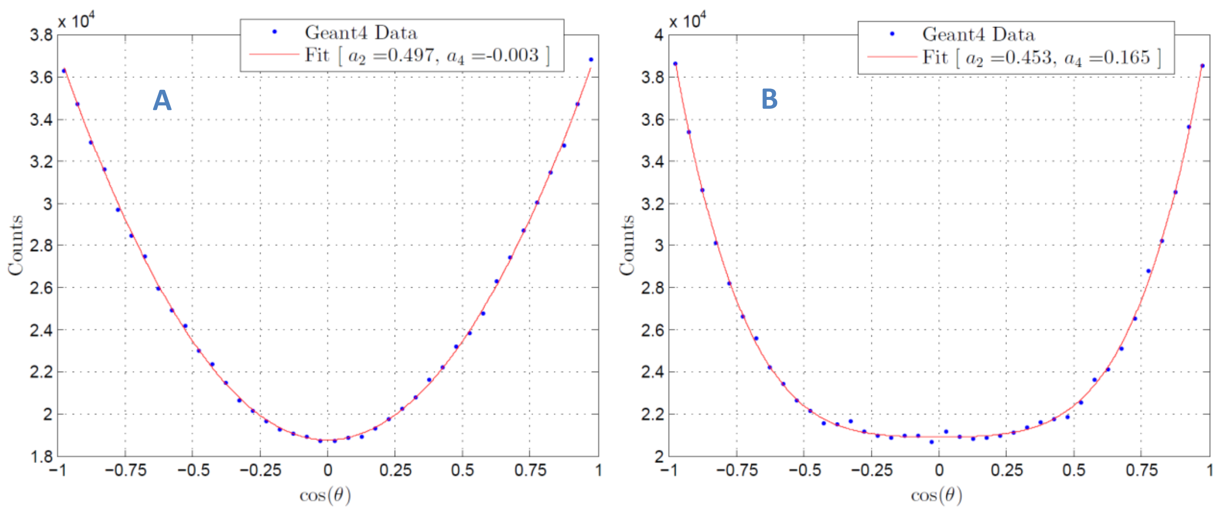


Figure 13 - Simulation and fit results of the correlation of the: [A] 100 and 200 keV gamma-rays. [B] 300 and 400 keV gamma-rays.

4. Geant4 Physics of Gamma-Gamma Correlations

In the original version of the radioactive decay module, the gamma-rays are emitted isotropically by default. In the gamma-gamma angular correlations extension of the radioactive decay code the gamma-ray cascade is tracked and the resulting gamma-rays are emitted relative to the gamma-ray that preceded it. If the gamma-ray being emitted in the excited daughter nucleus was feed directly via a beta decay (or any process which changes the A or Z of the nucleus), it is flagged as the first gamma decay, and will be emitted isotropically in 4π. The next gamma-ray will be emitted in a direction relative to the direction of the previous gamma-ray, and so on.

Consider the very general gamma-ray cascade in Figure 14.

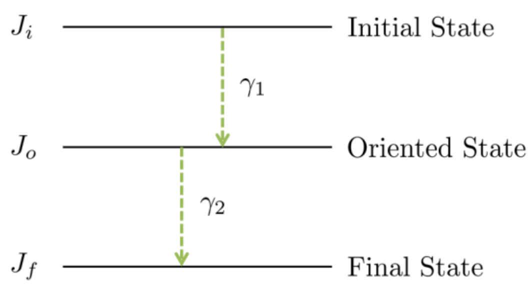


Figure 14 - Example gamma-ray cascade.

The correlation of the succeeding gamma-ray can be represented by the angular distribution function [2, 3, 4],

$$W(\theta) = 1 + a_2 P_2(\theta) + a_4 P_4(\theta) \, ,$$

where ϑ is the angle between the first and second gamma-rays, and P_2 and P_4 are Legendre polynomials. The angular correlation coefficients a_2 and a_4 are given by [2],

$$a_\lambda = B_\lambda(\gamma_1) A_\lambda(\gamma_2) \, ,$$

where B_λ is a function of the first gamma-ray and A_λ is a function of the second gamma-ray. They are defined as the following [2]:

$$B_\lambda(\gamma_1) = \frac{F_\lambda(L_1 L_1 J_i J_o) + (-1)^{L_1 + L_1'} 2\delta_1 F_\lambda\left(L_1 L_1' J_i J_o\right) + \delta_1{}^2 F_\lambda\left(L_1' L_1' J_i J_o\right)}{1 + \delta_1{}^2}$$

$$A_\lambda(\gamma_2) = \frac{F_\lambda\left(L_2 L_2 J_f J_o\right) + 2\delta_2 F_\lambda\left(L_2 L_2' J_f J_o\right) + \delta_2{}^2 F_\lambda\left(L_2' L_2' J_f J_o\right)}{1 + \delta_2{}^2}$$

The F_λ coefficients can be calculated via Racah W and Clebsch-Gordan coefficients [3], which then can be represented in terms of 6 and 3-j symbols. This formation of the angular distribution function is very general, and permits mixing in both the first and second gamma-ray transitions.

This angular distribution is calculated for every possible transition in the Geant4 level scheme. It is important to note that the lowest excited state cannot be within 2 keV of the ground state (0 keV). This ensures we correctly identify the angular momentum of each state.

The radioactive decay module has the ability to simulate a chain of decays before reaching a stable nucleus. The gamma-gamma correlations extension preserves this ability, and the user can simulate a chain of many gamma-gamma correlated decays.

5. Future Directions

The best outcome of this work would be for the gamma-gamma correlations code to be accepted by the Geant4 collaboration and included in future releases of Geant4. In that scenario, there would most likely not be a need for the multipole input file. Simply adding two more columns to the photon evaporation input file will provide enough information to include gamma-gamma correlations into Geant4.

6. References

1. S. Incerti et al, *Int. J. Model. Simul. Sci. Comput.* 1 (2010) 157–178

2. Paul D. Schmelzenbach. *The Study of 150Sm Through the Beta Decay of 150Pm, 150mEu and 150gEu.* Ph.D. Thesis, Oregon State University, Corvallis, Oregon, United States, 2003.

3. T. Yamazaki. *Nuclear Data A*, 3(1):1–23, 1967.

4. H. A. Tolhoek and J. A. M. Cox. *Physica*, 19:101–119, 1953.