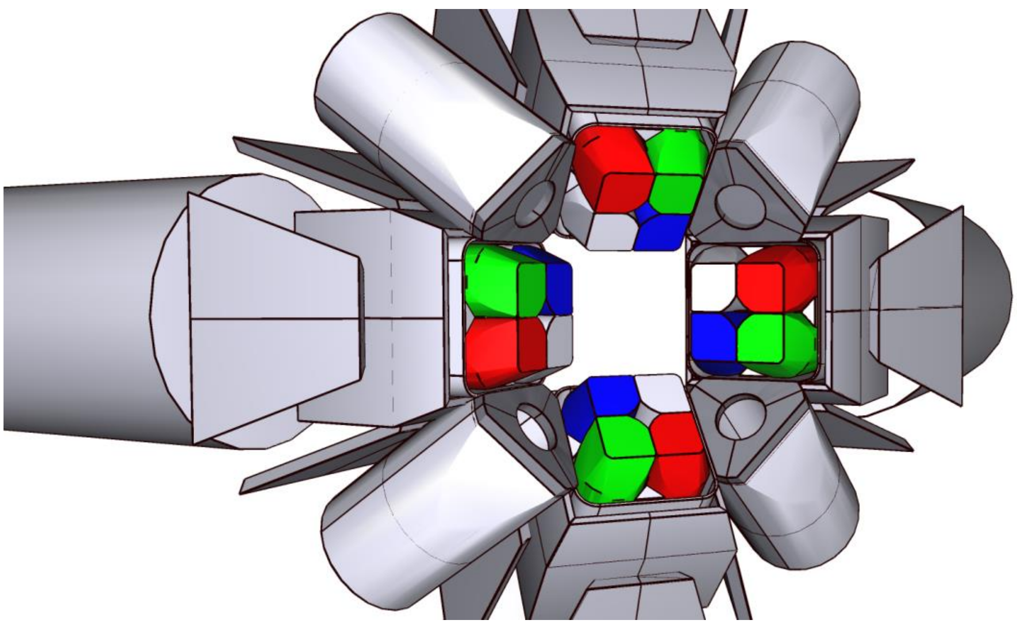
THE UNIVERSITY OF GUELPH

Geant4 Gamma-Gamma Angular Correlations (GGAC)

Geant4 Version 10.1



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This document outlines the capabilities and operation of the gamma-gamma angular correlations (GGAC) code in Geant4. The code responsible for the GGAC was written as an extension to the existing radioactive decay module in Geant4.10.1.

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 Geant4 [1] simulations outlined in this document were run on the Geant4 virtual machine provided by the IN2P3 group [2]. The gamma-gamma angular correlations code has been tested on the most recent version of Geant4 version 10.1.

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 painfully 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

The gamma-gamma angular correlations (GGAC) code is a small extension the existing radioactive decay module. The user has full control whether to use or not use the GGAC extension. If the user chooses not to use GGAC in his/her simulation, simply run the radioactive decay module as normal and the gamma-rays will be emitted isotopically in space. If the user chooses to use GGAC, two additional inputs are required on top of the typical radioactive decay input. The first required 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. See Section 3 for more detail on how to run simulations using GGAC.

2. Installing Gamma-Gamma Correlations Extension

The GGAC code has been appended onto the existing radioactive decay and photon evaporation code, and consequently, includes **no** new classes in the source code of Geant4. The GGAC 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 GGAC 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/geant4.10.01/source/processes/hadronic/models/…
radioactive_decay/
/usr/local/src/geant4.10.01/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

Before we get into the details of the GGAC extension to the radioactive decay module, let us run a simple example without GGAC. We will use the same Geant4 simulation to run simulations of the decay of ^{60}Co with and without GGAC. Packaged with this document should be an example Geant4 simulation *rdecay01_ggac*. This simulation is a modified version of the example simulation *rdecay01.* The *rdecay01* simulation is provided by the Geant4 collaboration and can be found in the following directory:

```
/usr/local/geant4.10.01/share/Geant4-10.1.0/…
examples/extended/radioactivedecay/rdecay01
```

The GGAC version (*rdecay01_ggac*) of this simulation differs as it includes a SteppingAction class to keep track of the cascading gamma-rays in a particular decay (in this case the gamma-rays emitted from the decay of ^{60}Co). This simulation also includes a histogram of the correlation between the two gamma-rays. To use this simulation with other decays please edit the SteppingAction.cc file to suit your needs.

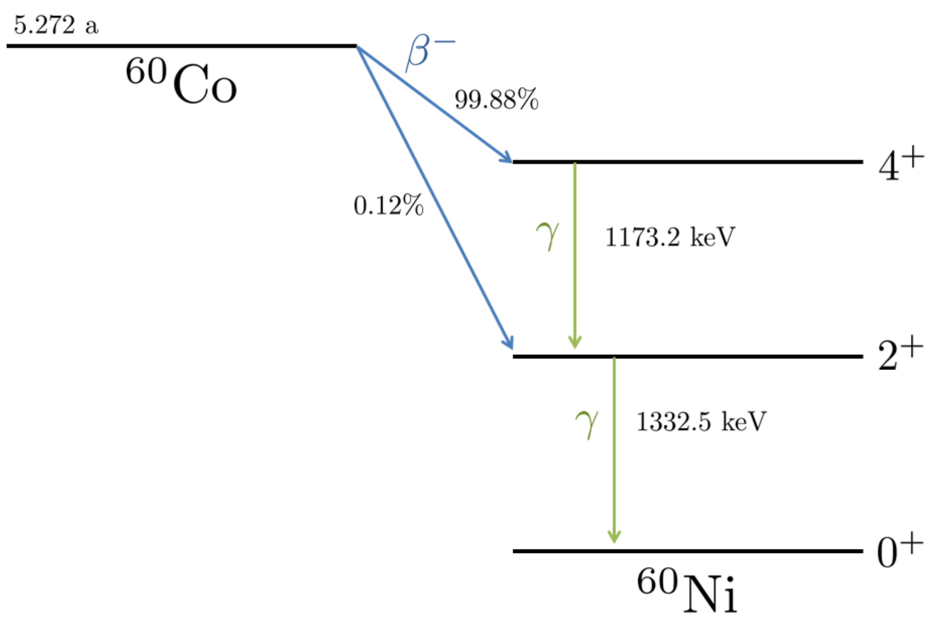


Figure 1 - Decay of ^{60}Co to ^{60}Ni.

Example 1

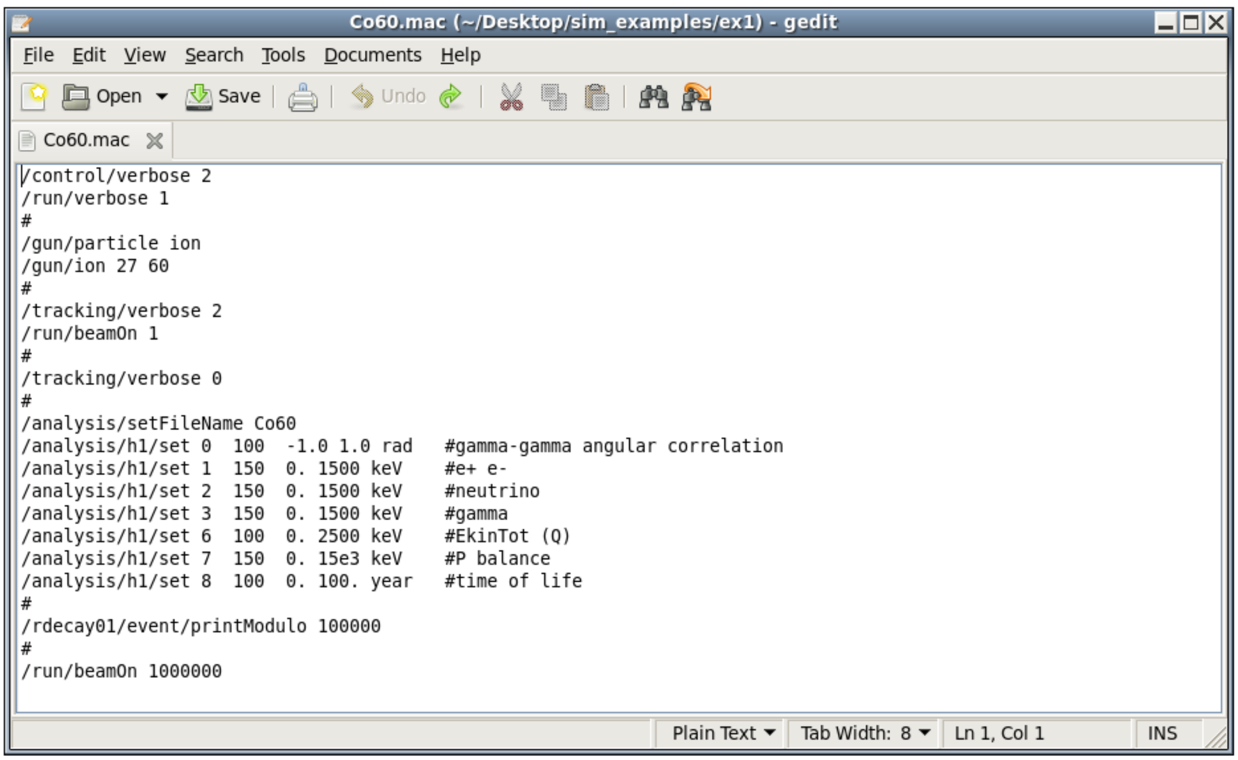
In these examples we will use a run macro provided in the *rdecay01* simulation and modify it to our needs. Copy the Co60.mac to your personal simulation directory, the Co60.mac file can be found in the *rdecay01_ggac* directory or from the following path:

```
/usr/local/geant4.10.01/share/Geant4-10.1.0/…
examples/extended/radioactivedecay/rdecay01/Co60.mac
```

Open the file and we'll want to add the following line where the histograms are defined:

```
/analysis/h1/set 0  100  -1.0 1.0 rad     #gamma-gamma angular correlation
```

This line defines the properties of histogram "0", which is the gamma-gamma correlation plot. The resulting macro file should look like Figure 2.




```
/control/verbose 2
/run/verbose 1
#
/gun/particle ion
/gun/ion 27 60
#
/tracking/verbose 2
/run/beamOn 1
#
/tracking/verbose 0
#
/analysis/setFileName Co60
/analysis/h1/set 0  100  -1.0 1.0 rad   #gamma-gamma angular correlation
/analysis/h1/set 1  150  0. 1500 keV    #e+ e-
/analysis/h1/set 2  150  0. 1500 keV    #neutrino
/analysis/h1/set 3  150  0. 1500 keV    #gamma
/analysis/h1/set 6  100  0. 2500 keV    #EkinTot (Q)
/analysis/h1/set 7  150  0. 15e3 keV    #P balance
/analysis/h1/set 8  100  0. 100. year   #time of life
#
/rdecay01/event/printModulo 100000
#
/run/beamOn 1000000
```

Figure 2 - Macro file for the decay of 60Co.

If we run this macro with the *rdecay01_ggac* simulation a root file is generated (Co60.root) as the output. If we open this root file and look at histogram 0 you'll notice there is no correlation between the two gamma-rays in ^{60}Ni (See Figure 3).

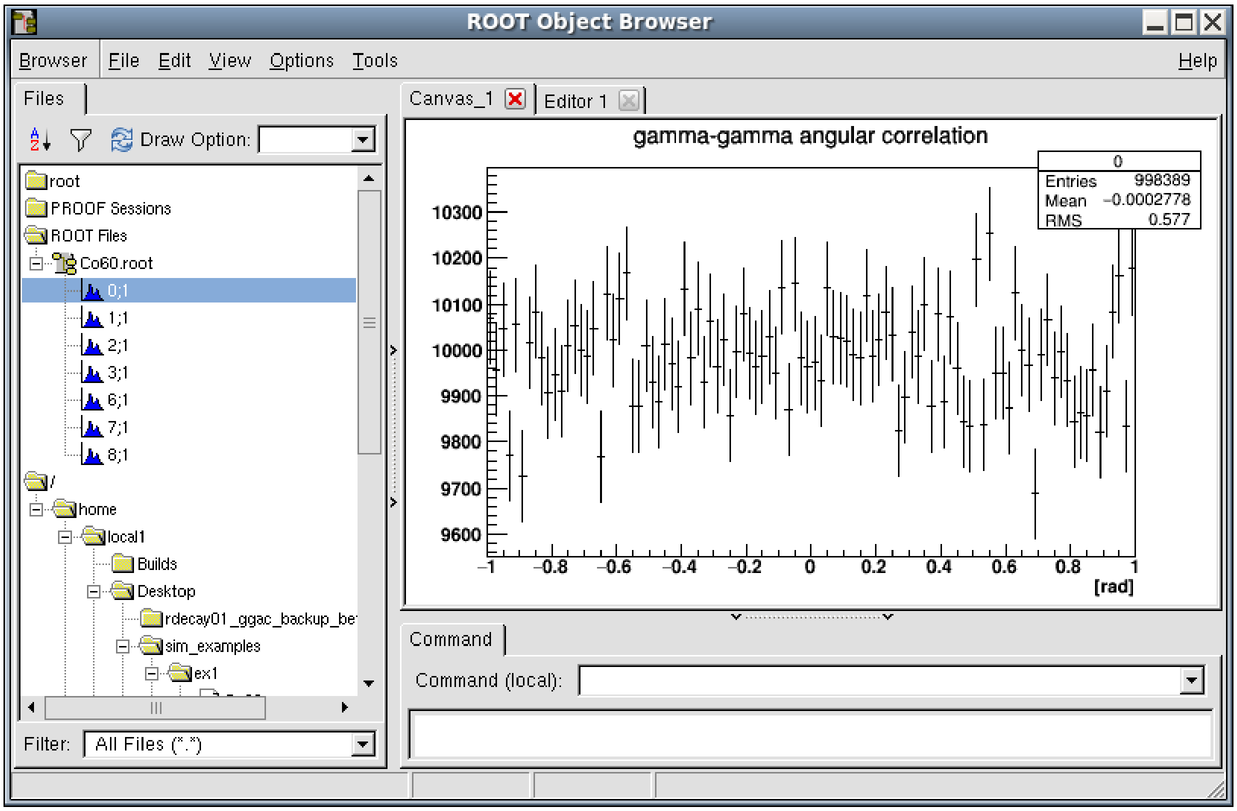


Figure 3 - Gamma-gamma correlation plot from the output file Co60.root.

In this example we did not include GGAC, additionally we did not define the properties of the ^{60}Co decay. We simply told Geant4 that our particle gun was an ion with a Z of 27 and an A of 60. During runtime the simulation looked up the data files for ^{60}Co and simulated the decay from these files. In many cases however, we would like to modify the properties of the decay. For example, we may have more information than what is provided in the Geant4 data files. In the next example we run the same simulation but directly supply the decay files.

Example 2

This example we will use the Co60.mac macro file from the previous example and we'll slightly modify it again. The first thing we need to do is make a new folder in our simulation directory. This folder is often named *UserData,* and it contains the data files which define the properties of the decay*.* We need to copy two files into this directory, the radioactive decay file and the photon evaporation file.

The radioactive decay files can be found in the following directory:

```
/usr/local/geant4.10.01/share/Geant4-10.1.0/…
data/RadioactiveDecay4.2/
```

For a complete description of the radioactive decay files please refer to the readme file *README_RDM* in the above path. We need the decay file for ^{60}Co, copy the file z27.a60 in your *UserData* folder. Let's rename this data file to UserRadData_z27.a60.

The photon evaporation data files can be found in the following directory:

```
/usr/local/geant4.10.01/share/Geant4-10.1.0/…
data/PhotonEvaporation3.1/
```

For a complete description of the photon evaporation data files please refer to the readme file *README-LevelGammaData* in the above path. We need the data file which contains the levels and gamma-rays in ^{60}Ni (Not ^{60}Co), copy the file z28.a60 in your *UserData* folder. Let's rename this data file to UserEvapData_z28.a60.

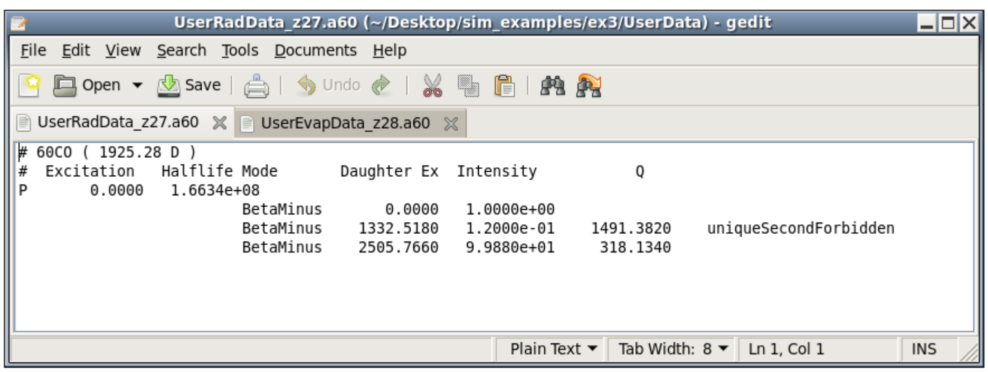


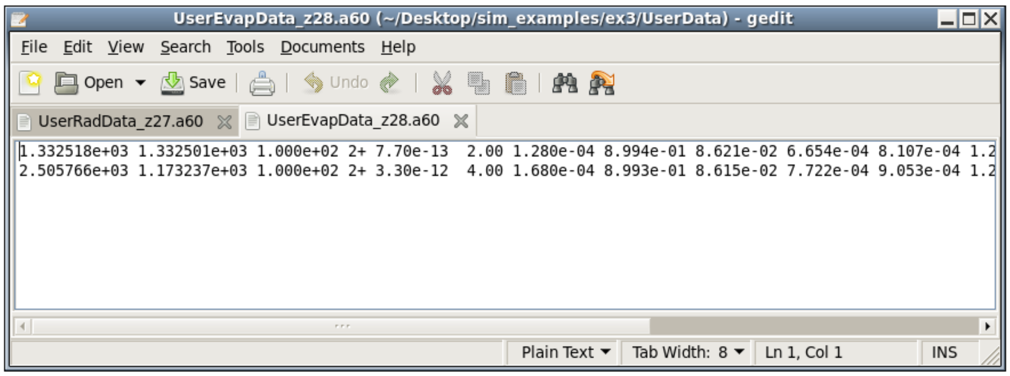
Figure 4 - Radioative decay file for 60Co.

The radioactive decay file and the photon evaporation files should look similar to Figures 4 and 5, respectively. In this example we have modified the data files to be a "simple" ^{60}Co decay, only 3 levels including the ground state and two gamma-rays. Now we can run our simulation with these input files. Open the run macro (Co60.mac) and insert the following two lines above the section that defines the "gun" properties:

```
/grdm/setRadioactiveDecayFile 27 60 UserData/UserRadData_z27.a60
/grdm/setPhotoEvaporationFile 28 60 UserData/UserEvapData_z28.a60
```

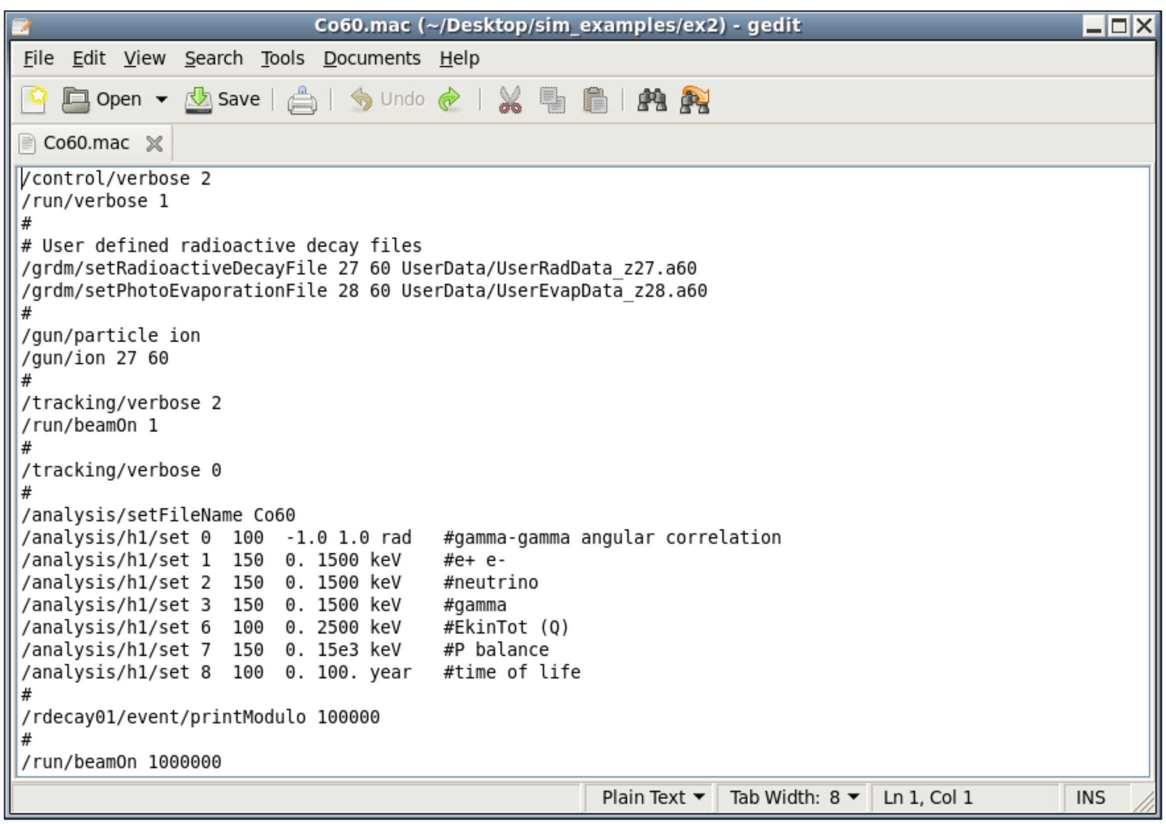
These commands require the Z of the nucleus, the A of the nucleus, and the location of the data file as input. The input macro file should look like Figure 6.

If we run this macro file we should get the same results as Example 1, but now we have full control of the decay properties through the radioactive decay and photon evaporation data files.




```
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 1.2
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 1.2
```

Figure 5 - Photon evaporation file for 60Ni.




```
/control/verbose 2
/run/verbose 1
#
# User defined radioactive decay files
/grdm/setRadioactiveDecayFile 27 60 UserData/UserRadData_z27.a60
/grdm/setPhotoEvaporationFile 28 60 UserData/UserEvapData_z28.a60
#
/gun/particle ion
/gun/ion 27 60
#
/tracking/verbose 2
/run/beamOn 1
#
/tracking/verbose 0
#
/analysis/setFileName Co60
/analysis/h1/set 0  100  -1.0 1.0 rad   #gamma-gamma angular correlation
/analysis/h1/set 1  150  0. 1500 keV    #e+ e-
/analysis/h1/set 2  150  0. 1500 keV    #neutrino
/analysis/h1/set 3  150  0. 1500 keV    #gamma
/analysis/h1/set 6  100  0. 2500 keV    #EkinTot (Q)
/analysis/h1/set 7  150  0. 15e3 keV    #P balance
/analysis/h1/set 8  100  0. 100. year   #time of life
#
/rdecay01/event/printModulo 100000
#
/run/beamOn 1000000
```

Figure 6 - Macro file for the decay of 60Co.

To run the GGAC 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 in the run macro, 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 the GGAC code. 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 "L_1" and the second column is "L_2". The last column is the mixing ratio (δ). For example, if the gamma-ray transition has a pure, unmixed, multipolarity only L_1 is needed. In this scenario L_2 and delta are set to zero. If the transition is mixed, consider an M1+E2 transition, then L_1 is set to 1 and L_2 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.

In the next example, Example 3, we will include the input require for GGAC.

Example 3

This example we will use the Co60.mac macro file from the previous example and we'll modify it again. Firstly we need to make the "Multipole" file in the *UserData* folder as described above. For two pure E2 transitions between the 4^+ to 2^+, and the 2^+ to 0^+, the multipole file should look like Figure 7.

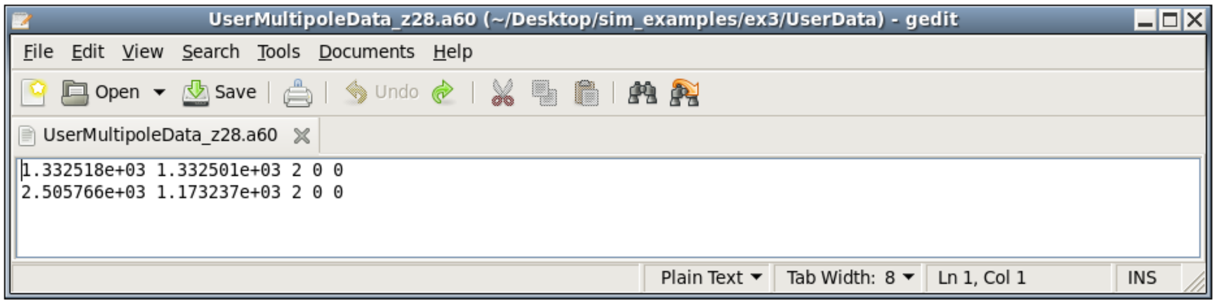


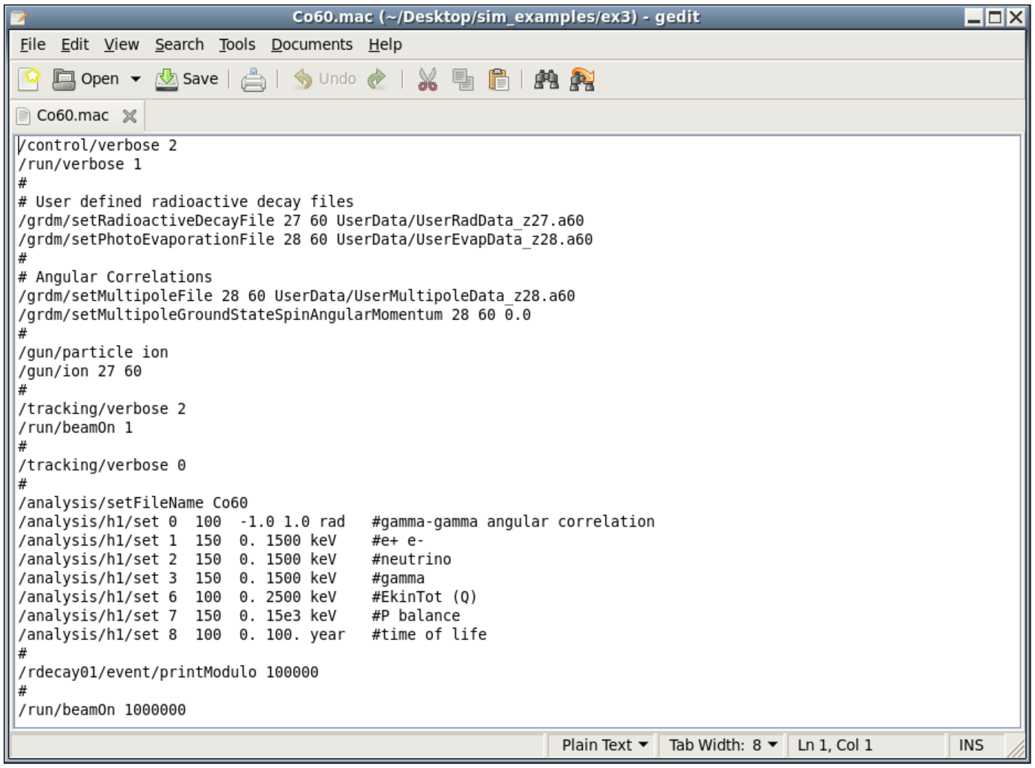
Figure 7 - Multipole file for 60Ni.

Now we need to modify the run macro to include this multipole file, as well as the spin of the ground state of the daughter nucleus. Immediately below where we set the radioactive decay and photon evaporation data files, include the following commands:

```
/grdm/setMultipoleFile 28 60 UserData/UserMultipoleData_z28.a60
/grdm/setMultipoleGroundStateSpinAngularMomentum 28 60 0.0
```

The first command is similar to the photon evaporation command and requires the Z of the nucleus, the A of the nucleus, and the location of the data file. The next command and requires the Z of the nucleus, the A of the nucleus, and the spin of the ground state of the daughter nucleus.

If we run this macro the resulting histogram 0 should look like Figure 9. Figure 9 is the angular correlation of the 1173.2 and 1332.5 keV gamma-rays for 10^6 decays of ^{60}Co. We can, of course, get better statistics by increasing the number of decays via the `beamOn` command in the macro file. Figure 10 [left] shows the result of 1 billion decays of ^{60}Co, fit using a Levenberg-Marquardt algorithm in Matlab. . Figure 10 [right] shows the result of 1 billion decays of ^{60}Co where the spin of the 2505.8 keV level was changed from 4+ to 0+. The decay is thus $0^+ \rightarrow 2^+ \rightarrow 0^+$, with both transitions being pure E2 transitions.



```
/control/verbose 2
/run/verbose 1
#
# User defined radioactive decay files
/grdm/setRadioactiveDecayFile 27 60 UserData/UserRadData_z27.a60
/grdm/setPhotoEvaporationFile 28 60 UserData/UserEvapData_z28.a60
#
# Angular Correlations
/grdm/setMultipoleFile 28 60 UserData/UserMultipoleData_z28.a60
/grdm/setMultipoleGroundStateSpinAngularMomentum 28 60 0.0
#
/gun/particle ion
/gun/ion 27 60
#
/tracking/verbose 2
/run/beamOn 1
#
/tracking/verbose 0
#
/analysis/setFileName Co60
/analysis/h1/set 0  100  -1.0 1.0 rad   #gamma-gamma angular correlation
/analysis/h1/set 1  150  0. 1500 keV    #e+ e-
/analysis/h1/set 2  150  0. 1500 keV    #neutrino
/analysis/h1/set 3  150  0. 1500 keV    #gamma
/analysis/h1/set 6  100  0. 2500 keV    #EkinTot (Q)
/analysis/h1/set 7  150  0. 15e3 keV    #P balance
/analysis/h1/set 8  100  0. 100. year   #time of life
#
/rdecay01/event/printModulo 100000
#
/run/beamOn 1000000
```


Figure 8 - Macro file for the decay of 60Co.

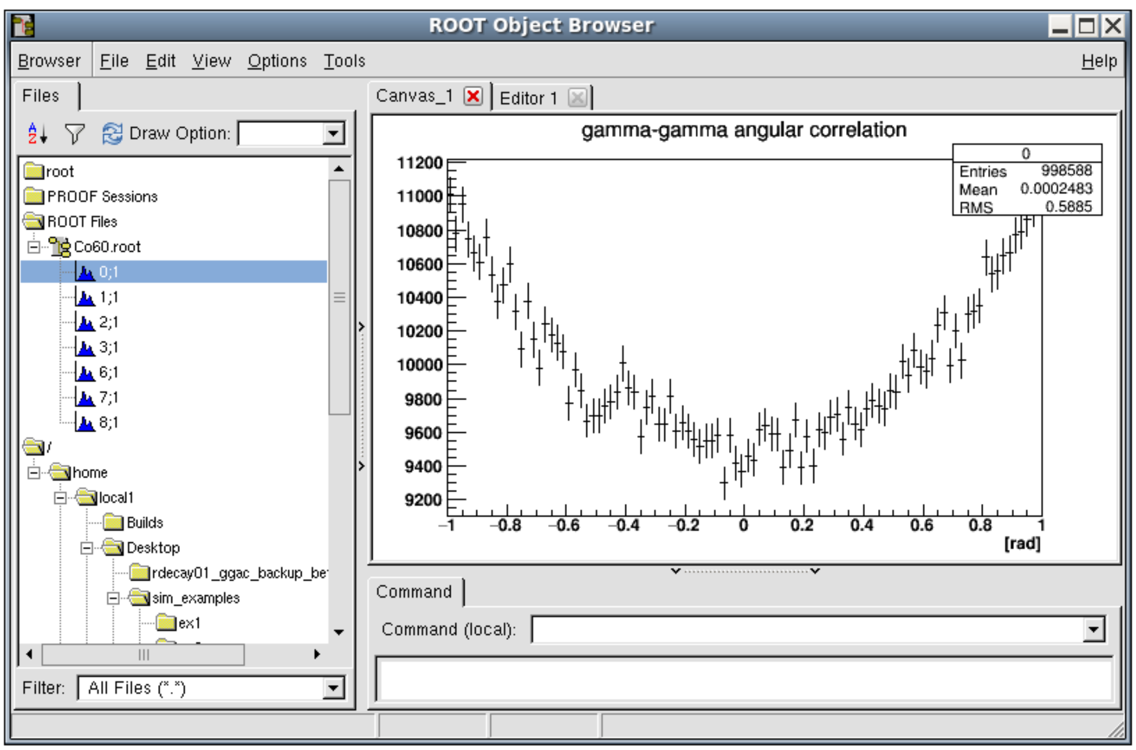


Figure 9 - Gamma-gamma angular correlation for the decay of ^{60}Co.

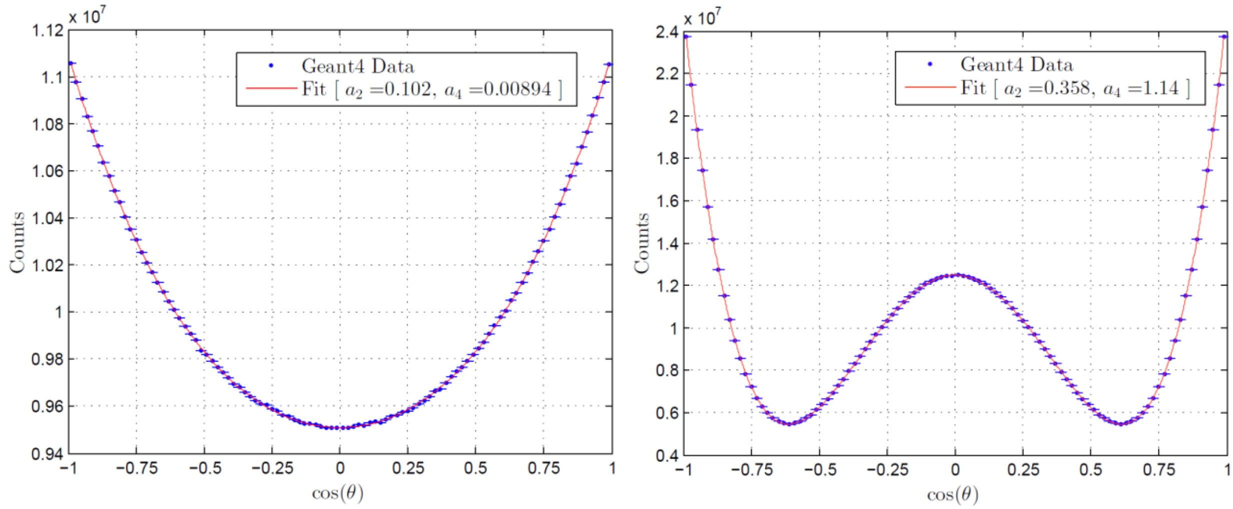


Figure 10 - [Left] 10^9 decays of ^{60}Co ($4^+ \rightarrow 2^+ \rightarrow 0^+$, both E2s). [Right] 10^9 decays of ^{60}Co ($0^+ \rightarrow 2^+ \rightarrow 0^+$, both E2s).

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 GGAC 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.

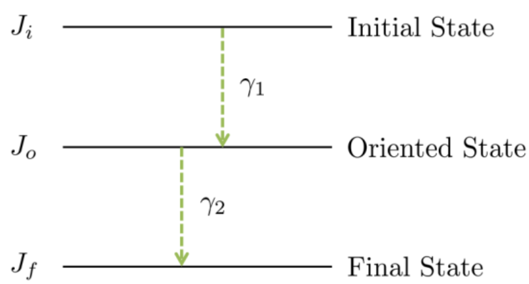


Figure 11 - Example gamma-ray cascade.

The correlation of the succeeding gamma-ray can be represented by the angular distribution function [3, 4, 5],

$$W(\theta) = 1 + \sum_{i=2,4,6,\ldots}^{2L} a_i P_i(\theta) \, ,$$

where ϑ is the angle between the first and second gamma-rays, and P_i are Legendre polynomials. The angular correlation coefficients a_2 and a_4 are given by [3],

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

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 [3]:

$$B_\lambda(\gamma_1) = \frac{F_\lambda(L_1 L_1 J_i J_o) + (-1)^{L_1+\acute{L}_1} 2\delta_1 F_\lambda(L_1 \acute{L}_1 J_i J_o) + \ {\delta_1}^2 F_\lambda(\acute{L}_1 \acute{L}_1 J_i J_o)}{1 + {\delta_1}^2}$$

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

The F_λ coefficients can be calculated via Racah W and Clebsch-Gordan coefficients [5, 6], 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.

The angular correlation coefficients are 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 GGAC into Geant4.

6. References

1. S. Agostinelli et al, *Nucl. Instr. Meth. A*, 506 (2003), 250–303

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

3. 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.

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

5. H. A. Tolhoek and J. A. M. Cox, *Physica*, 19 (1953), 101–119

6. L. Zuo et al, *J. Appl. Cryst.* 26 (1993) 302-119