# Angular Correlations Extension for Geant4

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# 1 Introduction

The angular correlation feature for Geant4, which previously handled only gamma-gamma correlations, has now been extended to include gamma-electron, electron-gamma, and electron-electron angular correlations. This report highlights the major changes made to the simulation code in order to achieve this. A sample simulation for the deexcitation of the 1048.5 keV, $I = 4^+$ excited state in Hg198 is also included. Finally, some further changes to the angular correlations feature are suggested.

## 1.1 Physics Background

All information for this section is taken from A.J. Becker and R.M. Steffen, *Physical Review*:180 [1].

The directional correlation of the radiation pair $R_1$ and $R_2$ is given by:

$$W(\theta) = \sum_{k \text{ even}} A_{kk} P_k(\cos\theta) \tag{1}$$

With the directional correlation coefficients being:

$$A_{kk} = A_k(R_1) A_k(R_2) \tag{2}$$

Depending on the type of radiation represented by $R_1$ (first transition) emitted from the nuclear state of angular momentum quantum number $I_1$ and $R_2$ (second transition) from the state $I_2$, the coefficients take a specific form. Below are the coefficients used when the first or second transition, respectively, emits a gamma ray. $I_3$ is the final state following the emissions.

$$A_k(\gamma_1) = \frac{F_k(L_1 L_1 I_1 I_2) + (-1)^{L_1 - L_1'} \times 2\delta(\gamma_1) F_k(L_1 L_1' I_1 I_2) + \delta^2(\gamma_1) F_k(L_1' L_1' I_1 I_2)}{1 + \delta^2(\gamma_1)} \tag{3}$$

$$A_k(\gamma_2) = \frac{F_k(L_2 L_2 I_3 I_2) + 2\delta(\gamma_2) F_k(L_2 L_2' I_3 I_2) + \delta^2(\gamma_2) F_k(L_2' L_2' I_3 I_2)}{1 + \delta^2(\gamma_2)} \tag{4}$$

Similarly, the coefficients used when the first or second transition emits an internal conversion electron are below; $b_k$ represents the internal conversion particle parameters.

$$\begin{aligned} A_k(e^-_{X1}) = \Big[ & b_k(\pi_1 L_1; X_1) F_k(L_1 L_1 I_1 I_2) + (-1)^{L_1 - L_1'} \times 2\delta(e^-_{X1}) b_k(\pi_1 L_1 \pi_1' L_1'; X_1) F_k(L_1 L_1' I_1 I_2) \\ & + \delta^2(e^-_{X1}) b_k(\pi_1' L_1'; X_1) F_k(L_1' L_1' I_1 I_2) \Big] \div \Big[ 1 + \delta^2(e^-_{X1}) \Big] \end{aligned} \tag{5}$$

$$\begin{aligned} A_k(e^-_{X2}) = \Big[ & b_k(\pi_2 L_2; X_2) F_k(L_2 L_2 I_3 I_2) + 2\delta(e^-_{X2}) b_k(\pi_2 L_2 \pi_2' L_2'; X_2) F_k(L_2 L_2' I_3 I_2) \\ & + \delta^2(e^-_{X2}) b_k(\pi_2' L_2'; X_2) F_k(L_2' L_2' I_3 I_2) \Big] \div \Big[ 1 + \delta^2(e^-_{X2}) \Big] \end{aligned} \tag{6}$$

Given the mixing ratios for the gamma transitions, the $\delta$ values for internal conversion can be determined by introducing the internal conversion coefficient $\alpha_X(\pi L)$ of the $(\pi L)$ multipole for electrons ejected from the $X$ shell:

$$\delta(e^-_{X1}) = \sqrt{\frac{\alpha_{X1}(\pi_1' L_1')}{\alpha_{X1}(\pi_1 L_1)}} \times \delta(\gamma_1) \tag{7}$$

$$\delta(e^-_{X2}) = \sqrt{\frac{\alpha_{X2}(\pi_2' L_2')}{\alpha_{X2}(\pi_2 L_2)}} \times \delta(\gamma_2) \tag{8}$$

# 2 Major Code Changes

Please note that many other changes were made to the code than outlined here. There will be more detailed documentation available in the future that will explain all changes, including the ones below.

## 2.1 G4NuclearLevel

The equations used to calculate the correlation coefficients $A_k(R_1)$ and $A_k(R_2)$ were re-written to the general forms in (5) and (6). These equations simplify to the pure $\gamma - \gamma$ case if the $b_k$ are set to 1 and the $e^-$ mixing ratios are set to the $\gamma$ mixing ratios. The coefficients $A_2, A_4, A_6, A_8$, and $A_{10}$ are calculated for the four possible deexcitation paths. These values are then output to the screen and saved so that they can be applied to generated particles as required. At the moment, $A_6$ to $A_{10}$ are set to zero. These higher order coefficients are small for the majority of nuclear transitions studied; in certain cases, their values are exactly zero and the $W(\theta)$ expansion containing only $A_2$ and $A_4$ is the complete solution. However, if the user does wish to calculate these higher order coefficients, she must input further $b_k$'s into the multipole file than are currently accepted (see Next Steps).

The output is now also surpressed for transitions with both $A_2$ and $A_4$ equal to zero, since these are not of interest to the user.

## 2.2 G4VGammaDeexcitation

This is where the gamma rays and electrons are generated, in accordance with the internal conversion coefficients. Once created, the particle type is accessed and the following tests are conducted to determine which type of correlation to apply to the particle.

- If the particle is the first one generated in the deexcitation process, its type is saved and the emission angle is randomly determined using a uniform distribution
- The correlation applied to the second and subsequent particles is determined in the following way:
  - Access the particle type of the previously generated particle
  - Access the current particle type
  - Based on the previous two definitions, set a case number for the particle pair
  - The case number is then passed to the function which will determine which correlation is applied to the current particle
  - Save the current particle's type as the "previous particle type" and repeat the entire process with the next product until the deexcitation is complete

With this method, the correlation applied to a specific particle depends only on the type of particle that was generated immediately before it (or is randomly set for the first product).

## 2.3 SteppingAction

For each new species that is simulated, the energy gates in this file must be reset. There are now four gates: two for each of the possible gamma transitions, and two for each of the possible electron transitions. Normally, a 1 keV window on each side of the expected energy is sufficiently narrow. For future extensions, keep in mind that Geant4 processes the products of deexcitation in a specific order. For example, all electrons are processed before all gammas, regardless of their position in the product list. Similarly, there is a hierarchy within both electrons and gammas which dictates that particles belonging to Transition 1 are always processed first. There is likely to be such a hierarchy when other particles (such as alphas and neutrinos) are involved in the deexcitation as well. It is therefore important to identify this hierarchy when making the changes to SteppingAction which decide when a certain transition of interest has been "found".

## 3 Sample Simulation

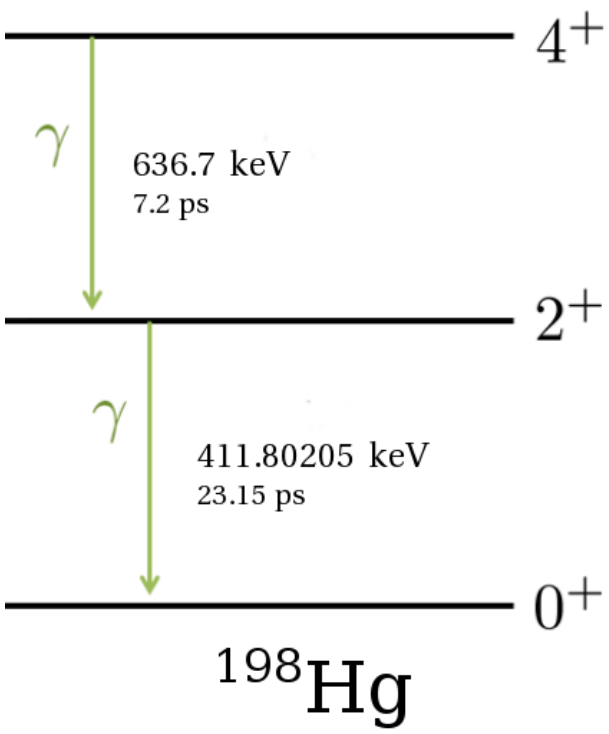


Figure 1: Deexcitation of $^{198}$Hg $4^+$

The next few pages contain the input to and result of the simulation for the $4^+ \rightarrow 2^+ \rightarrow 0^+$ (ground state) deexcitation of Hg198.

The K-electron shell binding energy for this species is 83.102 keV. With this information and the level scheme above [1], we know that:

- $\gamma_1$ has energy 636.7 keV
- $\gamma_2$ has energy 411.8 keV
- $e_1^-$ has energy 553.3 keV
- $e_2^-$ has energy 329 keV

Both electrons are from the K-shell.

[1] modified from [7]

Table 1: Multipole File Data

| | $E_x$ (keV) | $E_\gamma$ (keV) | $L$ | $L'$ | $\delta$ | $b_{2L}$ | $b_{2LL'}$ | $b_{2L'}$ | $b_{4L}$ | $b_{4LL'}$ | $b_{4L'}$ | $\alpha_K^L$ | $\alpha_K^{L'}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Second Transition | 411.8 | 411.8 | 2 | 0 | 0.0 | 1.44 | 0.0 | 0.0 | −0.10 | 0.0 | 0.00 | 0.0300 | 0.00 |
| First Transition | 1048.5 | 636.4 | 2 | 3 | 0.1 | 1.29 | 0.7 | 1.1 | 0.28 | 0.7 | 1.57 | 0.0117 | 0.2273 |

Table 2: Angular Coefficients

| Type | $A_2$ | $A_4$ |
|---|---|---|
| $\gamma\ \gamma$ | 0.158149 | −0.00398752 |
| $\gamma\ e^-$ | 0.227734 | 0.000398752 |
| $e^-\ \gamma$ | 0.218262 | −0.02440970 |
| $e^-e^-$ | 0.314298 | 0.002440970 |

Table 3: Branching Ratios

| Type | Simulation | Expectation |
|---|---|---|
| $\gamma\ \gamma$ | 94.36% | 95.96% |
| $\gamma\ e^-$ | 2.84% | 2.88% |
| $e^-\ \gamma$ | 1.11% | 1.12% |
| $e^-e^-$ | 0.033% | 0.034% |

$b_{2L}, b_{2LL'}$, and $b_{2L'}$ values were interpolated from [3] using linear regression. A graphical representation of the values used in the interpolations is below. $L$ is $E2$ and $L'$ is $M3$.

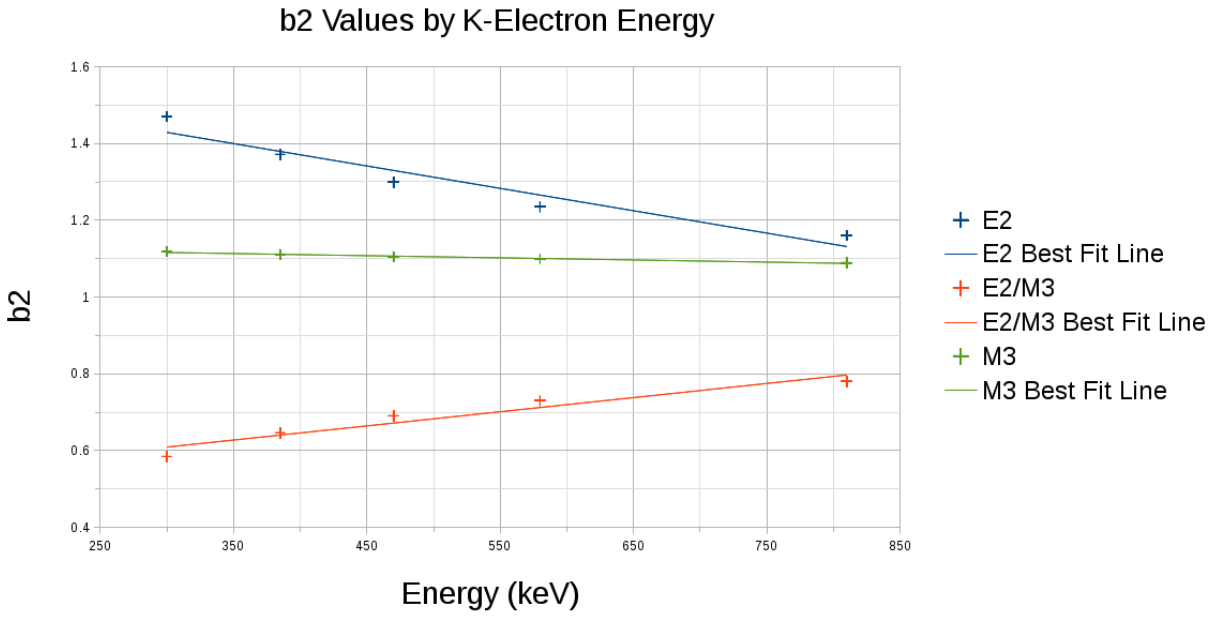


Figure 2: interpolated $b_2$ values

The higher order $b_4$ terms were determined using the recursive formula in [2].

$\alpha$ values are taken from BrIcc [5], and the mixing ratios $\delta$ were found in the nuclear data sheet for A = 198 [4]. The $\gamma - \gamma$ angular coefficients were compared with the values obtained from the GRIFFIN Angular Correlation Utility [6]. The coefficients calculated by the simulation matched those from the utility.

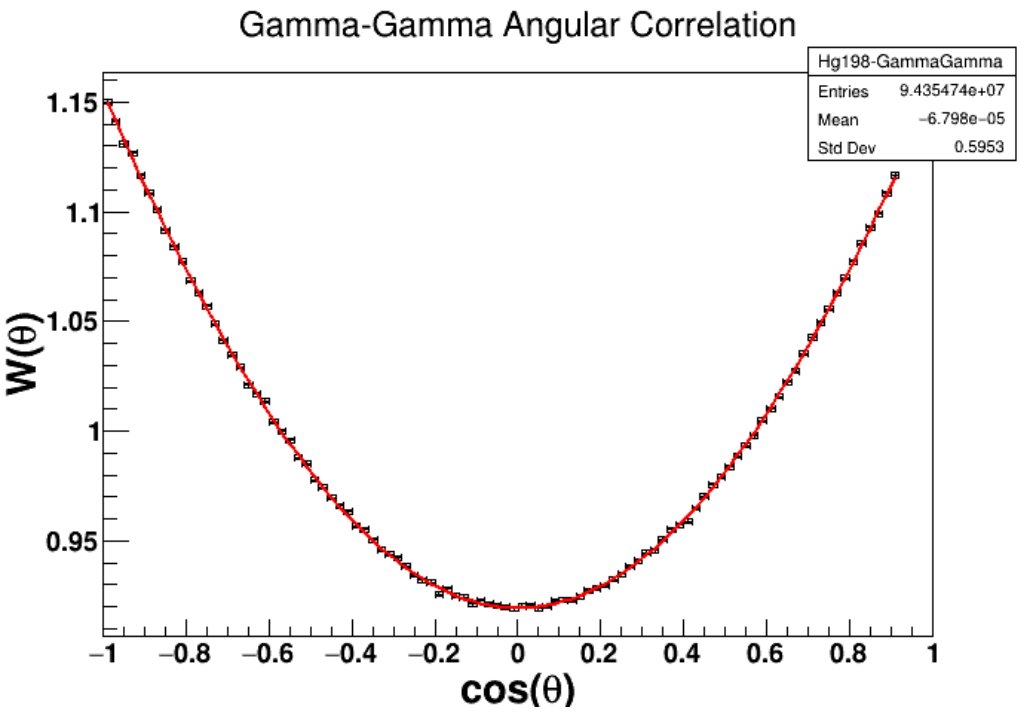


Figure 3: $\gamma - \gamma$ correlation for 100 million decays with theory line

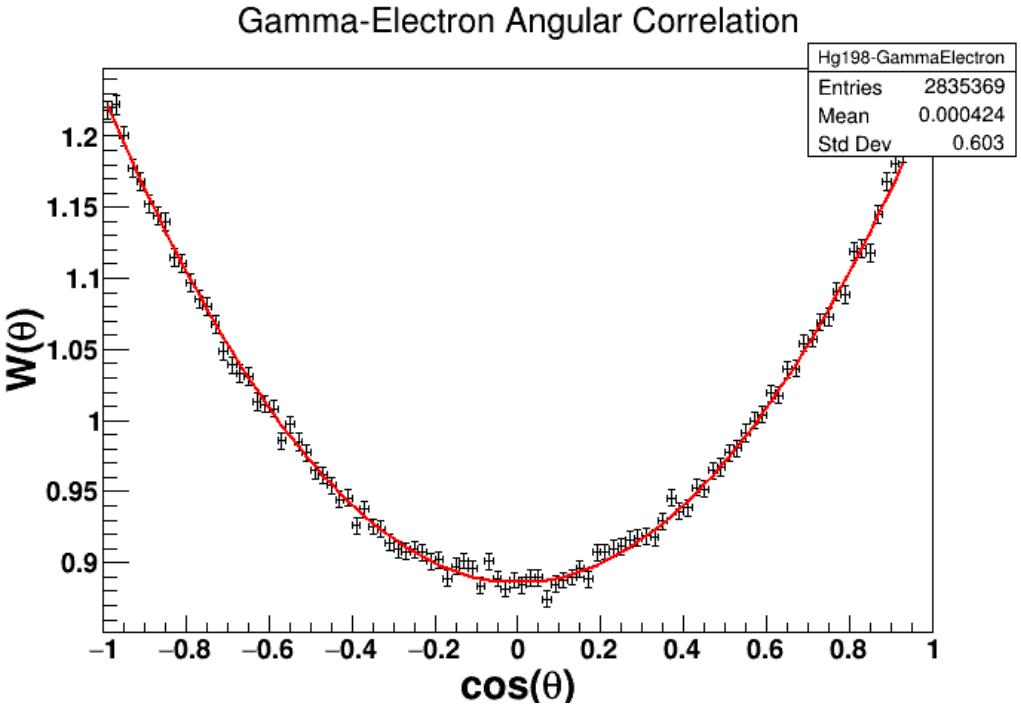


Figure 4: $\gamma - e^-$ correlation for 100 million decays with theory line

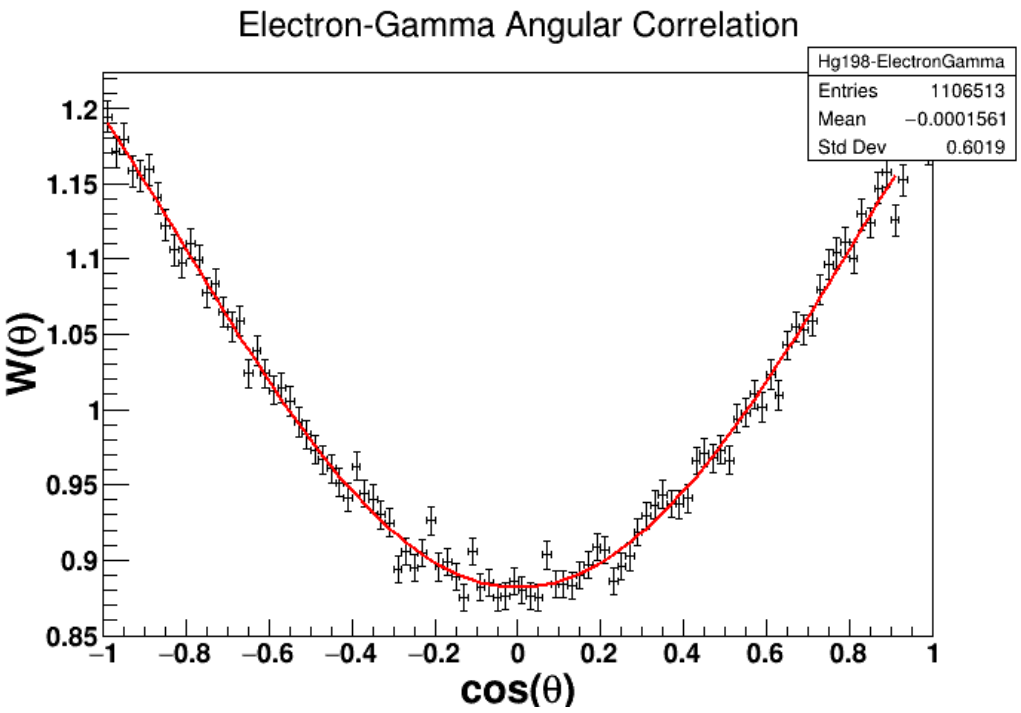


Figure 5: $e^- - \gamma$ correlation for 100 million decays with theory line

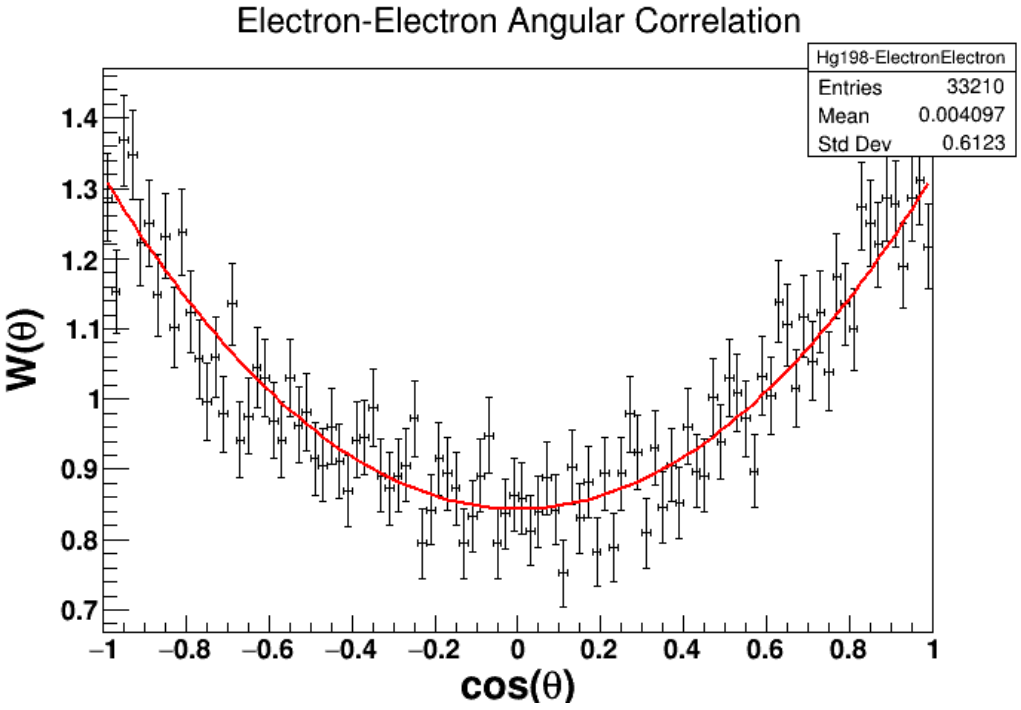


Figure 6: $e^- - e^-$ correlation for 100 million decays with theory line

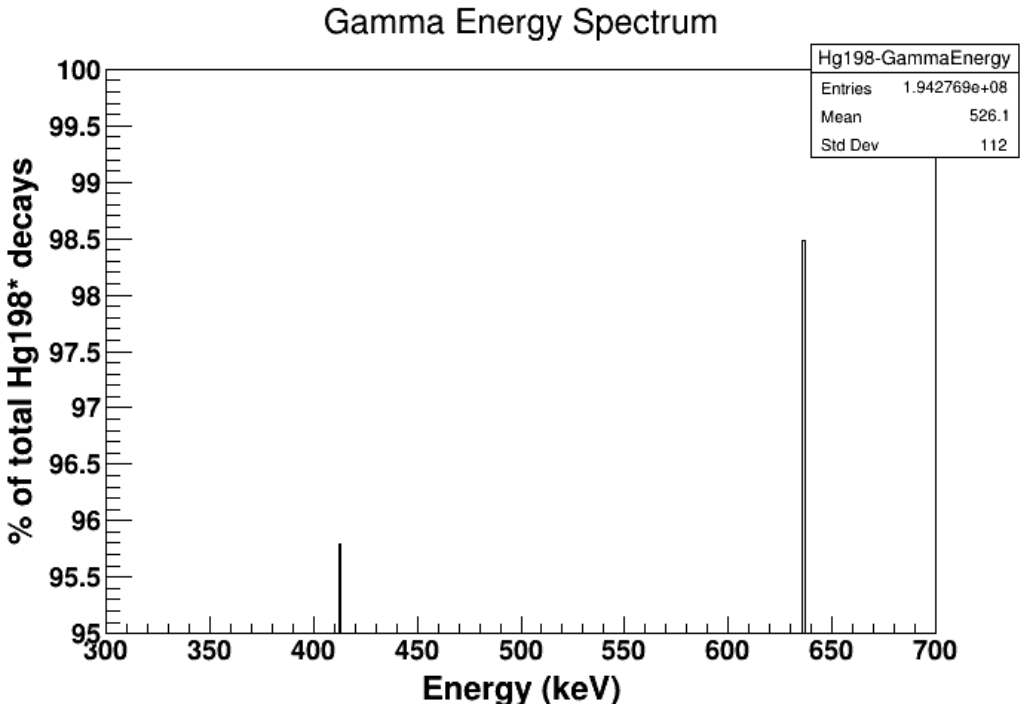


Figure 7: $\gamma$ energy spectrum for 100 million decays

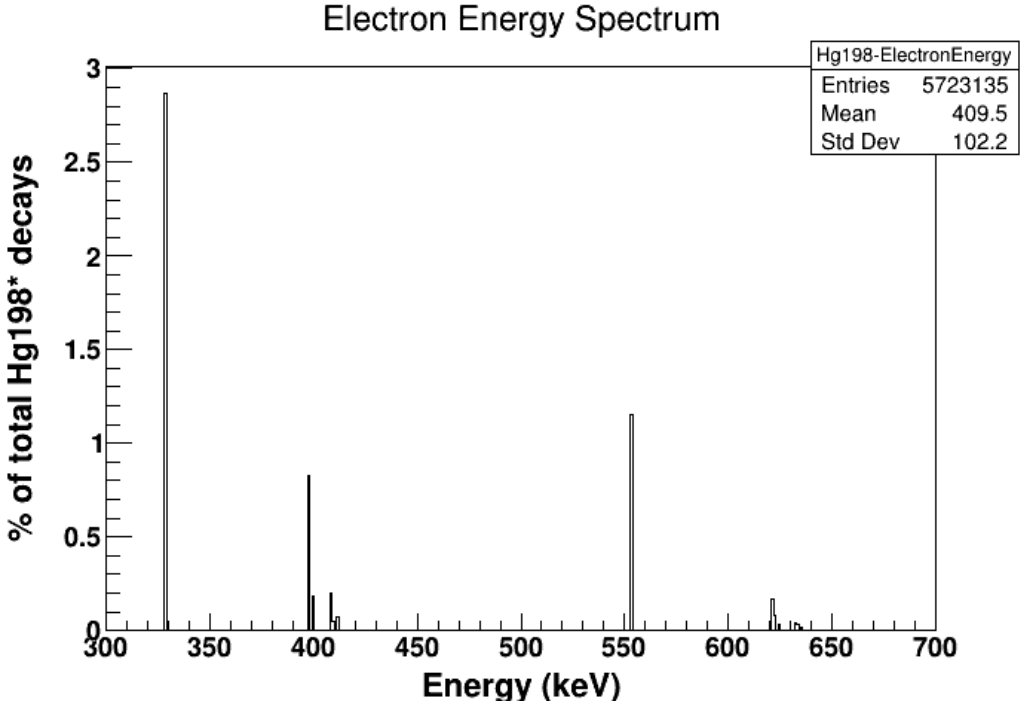


Figure 8: $e^-$ energy spectrum for 100 million decays

# 4 Next Steps

- These changes have only been made to the pure simulation; the detectors must also be taken into account. A detector simulation plot of gamma-gamma correlations has been completed by Anita Mathews, so plots for the remaining three transition types must be created (underway).
- The correlation plots produced by the simulation are oddly normalized. It seems that the shape of the graph was much more important than the scale of the y-axis when first developed. The normalization procedure needs to be updated to make sense of the y-axis. Currently, the $W(\theta)$ for each particle is randomly normalized using a uniform distribution.
- A feature exists to enter manual angular coefficients for the gamma-gamma case. It would be good to extend this manual entry to the other cases as well.
- The code only reads in $b_2$ and $b_4$ values from the multipole file. To get non-zero $A_6$ through $A_{10}$, the user needs to include the corresponding $b_k$ values in the multipole file, so the program must be extended to allow reading in of these extra values.
- It may be of interest to incorporate other particles (aside from just gammas and electrons) into the angular correlations extension. To do this, a lot more physics needs to be added to the base Geant4 code, including the various $A_k$ equations for different particles. See also the note in 2.3) SteppingAction.

# References


[1] A. J. Becker and R. M. Steffen. "$M1 - E2$ mixing ratios and conversion-electron particle parameters for the electromagnetic transitions in $As^{75}$". In: *Phys. Rev.* 180 (4 Apr. 1969), 1043–1048. DOI: 10.1103/PhysRev.180.1043. URL: https://link.aps.org/doi/10.1103/PhysRev.180.1043.

[2] R. Hager and E. Seltzer. "Internal conversion tables part II: Directional and polarization particle parameters for Z = 30 to Z = 103". In: *Nuclear Data Sheets. Section A* 4.5 (1968), pp. 397–411. ISSN: 0550-306X. DOI: https://doi.org/10.1016/S0550-306X(68)80017-5. URL: https://goo.gl/LkLTHP.

[3] R. Hager and E. Seltzer. "Table II directional particle parameters $b_k(L, L')$, for K-, L-, and M-shells, Polarization particle parameters $b_k^x(L, L'), b_k^y(L, L'), b_k^z(L, L')$, for K-shell". In: *Nuclear Data Sheets. Section A* 4.5 (1968), pp. 419–641. ISSN: 0550-306X. DOI: https://doi.org/10.1016/S0550-306X(68)80019-9. URL: https://goo.gl/JPtXJz.

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[5] T. Kibédi et al. "Evaluation of theoretical conversion coefficients using BrIcc". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 589.2 (2008), pp. 202–229. ISSN: 0168-9002. DOI: https://doi.org/10.1016/j.nima.2008.02.051. URL: https://goo.gl/QKgSg5.

[6] B. Mills and J. K. Smith. *Angular Correlation Utility: bugfixes, dep upgrades*. Feb. 2016. DOI: {10.5281/zenodo.45587}. URL: https://doi.org/10.5281/zenodo.45587.

[7] E. Rand. *Geant4 Gamma Gamma Angular Correlations README*. 2015. URL: https://git.io/vFK9v.