

# Gamma-ray and Electron Physics Processes in Geant

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To make sure that we were setting the physics interaction flags and the tracking cuts right for simulations of gamma rays from energy 180 keV to few MeV we wrote a simple Geant program called 'stop1'. Our previous experience with [Geant](#) has been limited to more than 100s of MeV so we felt it necessary to go through this exercise. This program is written to calculate the deposited energy spectrum in various material with varying thickness and a cross-sectional area of 10 cm X 10 cm. We also provided ourselves an option of placing an attenuator in front of the detector. [Geant](#) is able to simulate the dominant processes, which can occur in the energy range from 10 keV to 10 TeV for electromagnetic interactions. In this document we discuss how [Geant](#) treats the main gamma ray/electron interactions and what flags control these reactions and how we intend to set these flags. The [Geant](#) program is part of the [CERN program library](#). Fig. 1 shows the geometry of the stop1 program and tracks from 3MeV gamma interaction with BGO detector material.

3 MeV  $\gamma$  with pair production + multiple compton scatterings

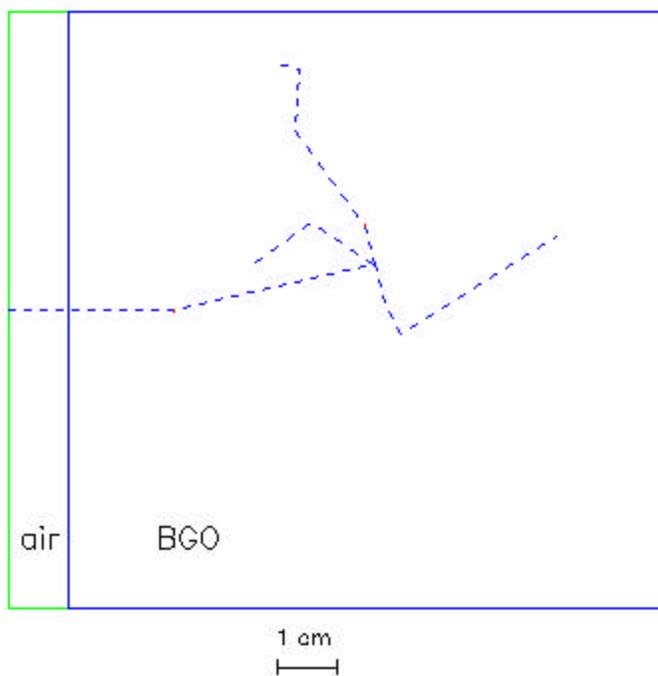


Fig. 1: Geometry used in stop1 program. Dotted lines indicate blue gamma tracks (dashes) and red tracks (solid lines) indicate electrons and positrons. Electron/positron track length is very small and sometimes cannot be seen in this picture.

## Photoelectric Effect<sup>i, ii</sup>

In a photoelectric interaction the gamma ray disappears and an electron appears with energy equal to  $E - Be$ , where  $Be$  is the binding energy of that electron and  $E$  is the energy of the incident gamma. The range of electrons in solid materials is so short that one can usually assume that all of the electron energy will be deposited. However if the interaction happens too close to the wall then the electron may deposit only part of its energy before escaping (the probability of this happening is very small). In practice one assumes that all of the energy of the photoelectron will be deposited in the detector. However this photoelectron energy is less than the gamma energy  $E$  by an amount  $Be$ . The atom is left in the excited state with excess energy of  $Be$ . The atom recovers its equilibrium in one of two ways. The atom may redistribute its excitation energy between its remaining electrons. This can result in release of further electrons from the atom (an Auger cascade), which transfers a further fraction of total gamma ray energy to the detector. Alternatively, an electron from higher energy level may fill the vacancy left by the ejection of photoelectron by dropping into it with the emission of characteristic X-ray, which is called X-ray fluorescence. This X-ray may then in turn undergo photoelectric absorption, perhaps emitting further X-rays, which are absorbed in turn until ultimately all the energy of the gamma ray is absorbed. When an electron is ejected from the atom, to conserve momentum some energy is lost to the recoiling atom. This recoiling energy is very small.

The energy level from which the electron is emitted depends on the energy of incident gamma ray. The most likely electron to be ejected is a K-shell electron (column 3 of the Table 1). If sufficient energy is not available to eject K electron then L and M electrons will be ejected instead. For the events near to the surface of the detector there is a reasonable probability that some fluorescent X-rays, most probably K X-rays, might escape from the detector. The net energy deposited in the detector is then  $E\gamma - E_{KX}$ , where  $E_{KX}$  is the energy of K X-ray of the detector material. This process is known as X-ray escape. Since precise amount of energy is lost, this gives rise to a definite peak at the low energy side of the full energy peak. Such peaks are prominent for thin detectors, high  $Z$ -detectors (e.g.  $\text{Bi}_4\text{Ge}_3\text{O}_{12}$  or [BGO](#),  $Z$  for Bi is 83, Density =  $7.13 \text{ gm/cm}^3$ ) and low energy gamma rays.

## Treatment of photoelectric effect in Geant<sup>iii</sup>

According to the Geant documentation, the photoelectric effect is treated as follows: If the energy of the radiation incident on an atom is  $E\gamma$ , then the quanta can be absorbed if  $E\gamma > E_{\text{shell}}$ . The photoelectron is emitted with total energy:

$$E_{\text{photoelectron}} = E\gamma - E_{\text{shell}} + m_e c^2$$

<sup>i</sup> W. R. Leo, "Techniques for Nuclear and Particle Physics Experiments: A How-to Approach," 2nd edition, 1994, Springer-Verlag.

<sup>ii</sup> Nicholas Tsoufanidis, "Measurement and Detection of Radiation," Second Edition, Taylor & Francis Ltd., (1995) p. 382 – 383.

<sup>iii</sup> CERN Program Library Long Write-up W5013, "GEANT: Detector description and simulations tool," Application Software Group Computing and Networks Division, CERN Geneva, Switzerland, 1993 (PHYS 231-1 & 2)

Probability of the interaction with an atom is calculated by taking into account partial cross-sections of atoms of a mixture or a compound. After this Geant calculates the probability of the interaction with a particular shell ( K, L<sub>I</sub>, L<sub>II</sub> and L<sub>III</sub>) of the chosen atom. For this Geant uses jump ratios<sup>iii</sup>. Using formulas given in the Geant manual we calculated the probability of the interaction with particular shell for few elements. Results for the nuclei used in materials in our TPC design are tabulated in Table 1. In this table we have not calculated the probabilities of the L<sub>II</sub> and L<sub>III</sub>. The equations used for calculating the probabilities of the four shells mentioned above add up to the total probability of 1.

Table I: The calculated probability of the photoelectric interaction with particular shell using Geant equations

Z	Element	Probability of the interaction with	
		K shell	L <sub>I</sub> shell
8	O	94.77%	0.87%
32	Ge	86.50%	2.25%
53	I	82.93%	2.84%
54	Xe	82.80%	2.87%
55	Cs	82.68%	2.89%
83	Bi	80.02%	3.33%

To be accurate the angular distributions of photoelectrons should be calculated using the partial wave analysis for the out-going electron. Since this method is very time consuming Geant uses approximations of the angular distributions calculated by F. von Sauter for K shell and Gavrilu for K and L shells. The cross-section approximation leads to zero scattering amplitude in the direction of incident gamma ray while experimentally the cross-section at zero degree angle is non-vanishing. After the photoelectron emission the atom is left in an excited state. The excitation energy is equal to the binding energy  $E_i$  of the shell in which the interaction took place. Subsequently the atom emits an X-ray gamma ray or Auger electron. The selection of radiative or non-radiative transition is based on cross-section compilation by Krause. The Auger transitions are represented by the most probable line for a given vacancy. The emitted electron energy  $E_e$

$$E_e = E_i - (E_j + E_k) \quad (1)$$

where  $E_i$ ,  $E_j$ ,  $E_k$  are the subshell binding energies and  $E_j > E_k$ . For emitted X-rays they use transition rates of Scofield. Geant only uses those transitions where the occurrence probability is greater than 1%. The X-ray photon is emitted with energy  $E_{\gamma'}$ , where  $E_{\gamma'} = E_i - E_j$  (2), for transition between the subshells  $i$  and  $j$ . In addition, to fulfill the energy conservation law, emission of an additional photon is simulated instead of simulating recoil of the atom. (In the Geant treatment of photoelectric effect it is assumed that the atom has an infinite mass.) For non-radiative transitions this emitted photon energy is  $E_k$  (see formula (1)). In case of X-ray transition this emitted photon energy is  $E_j$  (see equation (2)). Below in Fig. 2 we show particle tracks from an event. Here, an X-ray

particle escapes from the active detector, but the rest of the incident gamma ray energy is detected.

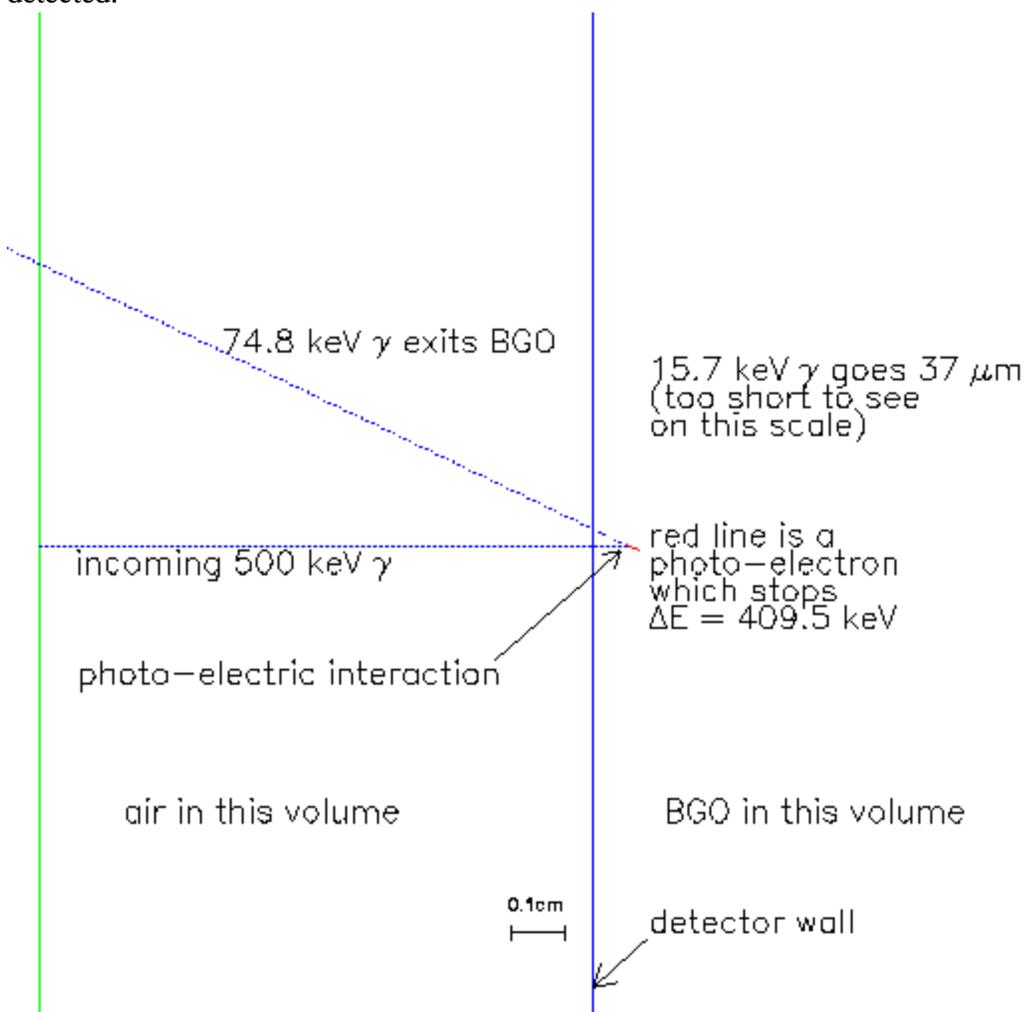


Fig. 2: Photoelectric interaction in GEANT.

The horizontal dotted line coming in from the left side of the picture represents an incoming 500 keV gamma ray. Near the center of the picture, there is a photoelectric interaction with Bi atoms in the BGO. Some useful cross-sections are shown in Table 2. These cross-sections were obtained using the commercial program [PHOTKOEFTM](#). This produces an electron (the short red track which goes down and to the right), a 75 keV photon from  $L_{II}$  ( $E_{\text{level}} = 15711.1$  eV)<sup>iv</sup> to K ( $E_{\text{level}} = 90525.9$  eV) transition of  $^{83}\text{Bi}$  (which goes up and to the left and eventually leaves the picture), and a 15.7 keV photon (which goes only 37 microns before "stopping").

<sup>iv</sup> CRC handbook of Chemistry and Physics, 81st edition, © 2001 Knovel.

Table 2. Photoelectric cross-section in barns at 500 keV and 1.5 MeV gamma rays on some nuclei.

E(keV)	Oxygen	Iodine	Cesium	Germanium	Bismuth
5.00E+02	5.63E-04	4.19E+00	4.94E+00	4.27E-01	2.99E+01
1.50E+03	5.05E-05	3.99E-01	4.74E-01	3.97E-02	3.03E+00

Because the particles do not all get very far from the vertex in this picture, here is a version that zooms in on the region around the vertex. In this plot the 15.7 keV photon can be seen:

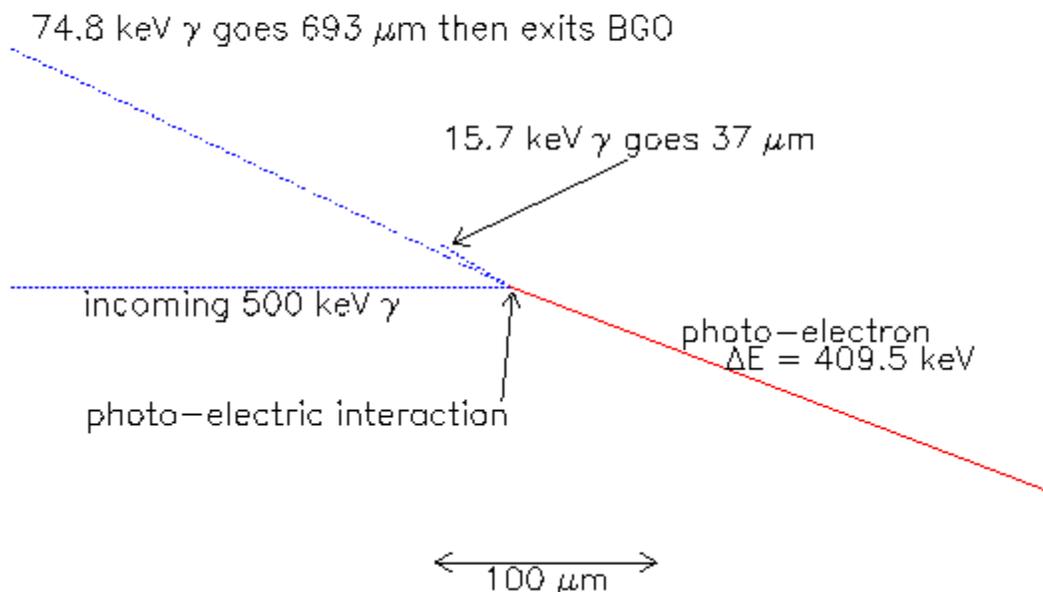


Fig. 3: Expanded version of the tracks shown in Fig. 2.

In this example, the 74.8 keV photon escapes from the system. This happens often enough to produce a sharp peak in the energy loss spectrum in the BGO at an energy corresponding to the photo-peak minus 74.8 keV when energy resolution is 0%. Fig. 2 and Fig. 3 were generated using the Geant drawing package (see manual for the details.) The interaction length used by Geant for the 15.7 keV photon in the example above is 13.6 microns and the interaction length for the 74.8 keV photon is 785 microns. However, the 74.8 keV electron only needs to go 693 microns to escape from the detector volume -- so in this case it does.

The IPHOT flag controls the photoelectric effect in Geant. It can be zero, which simply turns the effect off, 1 (default value) which works as described above, or IPHOT=2. If IPHOT=2, all the energy produced in the photoelectric interaction is deposited directly at the vertex without generation and transportation of electrons and X-rays. Since we are trying to model reconstruction of Compton-scattering using electron tracks, it is necessary for us to be able to tell the difference between photo-electric interaction and Compton interaction, so we did not want to use IPHOT=2.

## Compton Scattering

Compton scattering is a scattering of gamma rays on ‘free’ electrons. In reality electrons are bound in an atom. If the incident gamma ray energy is much greater than the binding energy of the electron then the binding energy can be ignored and electrons are considered to be ‘free’. The variable ICOMP controls this process. You can completely turn off this interaction using ICOMP =0. The default value of ICOMP is 1. At this value of ICOMP the Geant simulation proceeds as follows:

The quantum mechanical Klein-Nishina differential cross-section used in Geant is:

$$\Phi(E,E') = (X_0 n \pi r_0^2 m_e) / E^2 [(1/\epsilon) + \epsilon] [1 - (\epsilon \sin^2 \theta) / (1 + \epsilon^2)]$$

where,

$E$  = energy of the incident gamma ray,  $E'$  = energy of the scattered gamma ray,  $\epsilon = E/E'$ ,  $m_e$  = electron mass,  $n$  = electron density,  $r_0$  = classical electron radius,  $X_0$  = radiation length.

Assuming an elastic collision, the scattering angle  $\theta$  is defined by the Compton formula:  
 $E' = E m_e / [m_e + E (1 - \cos \theta)]$

Geant uses the combined “composition and rejection” Monte Carlo method for sampling of  $\epsilon$ . After the successful sampling of  $\epsilon$ , Geant generates the polar angles of the scattered gamma ray with respect to the direction of the parent gamma ray. The azimuthal angle,  $\phi$ , is generated isotropically and  $\theta$  is as defined above. The momentum vector of the scattered gamma ray is then calculated according to kinematic considerations. Both vectors are then transformed into the GEANT coordinate system. In Geant, the differential cross-section is only valid for those collisions in which the energy of the recoil electron is large compared with its binding energy (which is ignored). After the Compton interaction all of the generated secondaries are appropriately tracked. If ICOMP=2 Compton scattering proceeds without generation of electrons. For our simulations we have set ICOMP flag to 1 as we want to study the electron tracks from this interaction. Fig. 4 shows a Geant event where a 1.5 MeV incoming gamma interacted in the BGO with the Compton interaction generating an electron. The 671.8-keV electron goes 0.063 cm before stopping. The red track indicates electron and dashed blue lines indicate gamma rays.

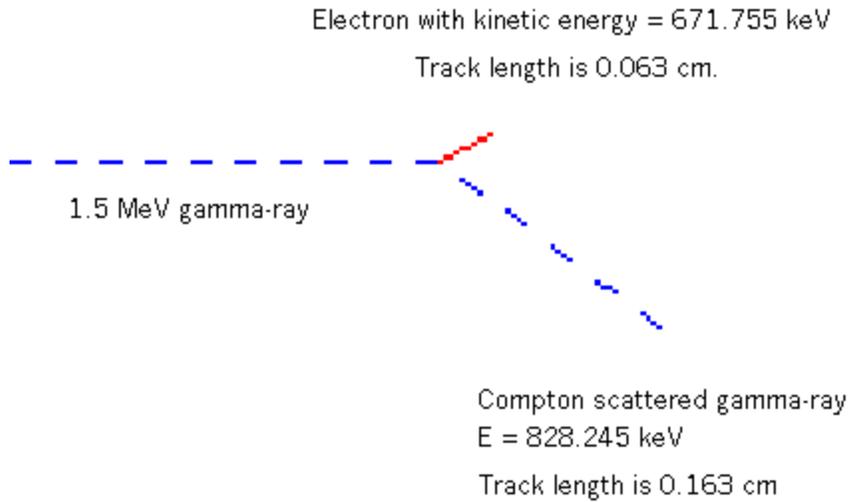


Fig. 4: Geant event showing a Compton interaction in BGO medium

## Pair Production

Here a gamma ray is converted into an electron-positron pair. In order to conserve momentum, pair production can only occur in the presence of a third body i.e. a nucleus or an electron. For this interaction to happen the incident gamma ray must have minimum energy of 1.022 MeV. (Note that pair production can take place in the field of an electron but the probability for that to happen is very small and the threshold for gamma-ray energy is 2.04 MeV.) The screening by the atomic electrons surrounding the nucleus plays important role in this interaction. In Geant the IPAIR flag controls this reaction. With IPAIR = 0 you can choose to turn off this interaction. For IPAIR = 1 Geant uses the Bethe-Heitler differential cross-section with the Coulomb correction for a gamma ray of energy E to produce a  $e^-e^+$  -pair with one of the particles having energy  $\epsilon E$  (is the fraction of the gamma ray energy carried by one particle of the pair) is given as

$$d\sigma(Z,E,\epsilon)/d\epsilon = r_0^2 \alpha Z [Z + \xi(Z)]/E^2 \{[\epsilon^2 + (1-\epsilon)^2][\Phi_1(\delta) - 0.5F(Z)] + (2/3)\epsilon(1-\epsilon)[\Phi_2(\delta) - 0.5F(Z)]\}$$

where  $\Phi_1(\delta)$  are screening functions depending on the screening variable  $\delta$ ,  $\alpha=1/137$ , and  $r_0$  = classical electron radius. For detailed description of the screening functions please look at the Geant manual. Effects due to the breakdown of Born approximation at low energies are ignored (but the Coulomb correction is included).

for very low energy gamma rays ( $E \ll 2.1$  MeV) the electron energy is approximated by sampling from a uniform distribution over the interval  $m \pm 1/(2E)$ .

For target materials composed of compounds or mixtures are treated identically to chemical elements (this is not the case when computing the mean free path!) using the effective atomic number computed. In Geant, the differential cross-section implicitly accounts for pair production in both nuclear and atomic electron fields. However, the recoil momentum of the target nucleus/electron is assumed to be zero. Fig. 5 shows a pair production event generated using Geant. The positron interacts with the NaI medium via annihilation interaction generating two gamma rays. For  $IPAIR = 2$  the interaction is considered but no electrons or positrons are generated. We will use  $IPAIR = 1$  for our calculations.

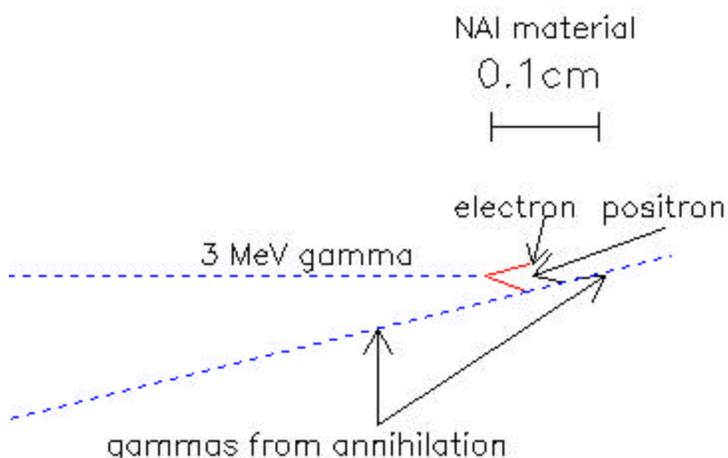


Fig.5: Pair production and annihilation interaction track. Incident gamma here had 3.0 MeV energy and the detector material was NaI. This figure was generated using GEANT program itself.

## Annihilation interaction

Positron generated in the pair production slows down and reaches the end of its range over a very short time (shorter than the time needed for pulse formation). Sometime before stopping but most of the time at the end of its track, it annihilates with an atomic electron. Most of the time two gamma rays are generated with combined energy equal to  $2m_e c^2$ , where  $m_e$  is the electron rest mass and  $c$  is the velocity of light. When annihilation happens after the  $e^+$  falls below the cutoff energy or stops, the gammas share an equal amount of energy i.e.  $m_e c^2$ . In this case the angular distribution of the emitted gamma rays is isotropic with gammas going in opposite directions. Positrons can also [annihilate to a single gamma ray](#) if the electron involved is bound in an atom.

If one annihilation gamma ray (out of two gamma rays generated) escapes from the medium then a pulse height proportional to energy  $(E - 0.511)$  MeV is observed, where  $E$  is the energy of the incoming gamma ray. Incident gamma rays who undergo pair production, followed by annihilation, then followed by escape of one gamma ray give rise to a single-escape peak at  $(E - 0.511)$  MeV, where  $E$  = energy of the incident gamma. Events in which both annihilation gamma rays escape, end up giving rise to a double-escape peak at  $(E-1.022)$  MeV.

Only a brief summary of the Geant treatment is given in this document. In Geant if the control flag IANNI is equal to 1 (default value) then the type of annihilation is sampled from the total cross-sections for the annihilation into two gamma rays and into one gamma ray. For the annihilation into two gamma rays the cross-section formula by Heitler is used. For compounds, the cross-section is calculated using an effective atomic number. In the derivation of the cross-section, only the interactions with the K-shell electrons are taken into account. As the cross-section depends on  $Z^5$ . The total cross-section for the positron annihilation is  $\sigma = \sigma_{2\gamma} + \sigma_{1\gamma}$ , where  $\sigma_{2\gamma}$  is the two photon annihilation cross-section. The value of  $\sigma_{1\gamma}$  (single photon annihilation cross-section) peaks at it largest for heavy materials, for example, it is ~20 % of the total cross-section for a positron of 440 keV kinetic energy in lead. For lower and higher energies the probability is lower. Annihilation into one gamma ray is treated as follows. The generated gamma ray is assumed to be collinear with the positron. Its energy will be,  $k = E + m_e - E_{\text{bind}}$ , where  $E_{\text{bind}}$  is the binding energy of the K-shell electron. Binding energy is estimated as follows,  $E_{\text{bind}} = 0.5(Z\alpha)^2 m_e$ , where  $\alpha$  is the fine structure constant.

In calculating the annihilation process it is assumed that the atomic electron initially is free and at rest. Also any higher order annihilation processes leading to generation of more than two gamma rays are not simulated in Geant. The variable IANNI controls this process. This interaction can be turned off by setting IANNI to zero. For IANNI = 2 it will consider the annihilation interaction but will not generate the secondaries. We need to use IANNI =1.

## Ionization by charged particles

Energy loss of charged particles is controlled by variable ILOSS. It is used in conjunction with  $\delta$ -ray production variable IDRAY.

ILOSS =0 No continuous energy loss, IDRAY is forced to 0 which means no  $\delta$ -rays are generated.

=1 Continuous energy loss with generation of  $\delta$ -rays above DCUTE (set to 1E4 GeV) and restricted Landau fluctuations below DCUTE .

=2 (Default value ) Continuous energy loss without generation of  $\delta$  -rays and full Landau-Vavilov-Gauss fluctuations. In this case the variable IDRAY is forced to 0 to avoid double counting of fluctuations.

=3 Same as 1, kept for backward compatibility.

=4 Energy loss without fluctuation. The value obtained from the tables is used directly.

For details about how different energy loss is calculated please see the Geant manual. For or detector we need to set ILOSS to 2 and IDRAY to 0.

## Bremsstrahlung

The variable IBREM controls this process. As usual

IBREM =0 No bremsstrahlung.

= 1 (Default value) bremsstrahlung with generation of  $\gamma$ .

=2 bremsstrahlung without generation of  $\gamma$ .

Every free charged particle that accelerates or decelerates loses part of its kinetic energy by emitting electromagnetic radiation. This radiation is called Bremsstrahlung. The Geant generates a bremsstrahlung photon from an electron as a discrete process. The photon energy is sampled from a parameterization<sup>v</sup> of the bremsstrahlung cross-section of Seltzer and Berger for electron energies below 10 GeV, and from the screened Bethe-Heitler cross-section above 10 GeV. Midgal corrections are applied in both cases. We have set IBREM to 1.

## Multiple scattering

The variable IMULS controls this process.

IMULS =0 No multiple scattering.

=1 (Default) Multiple scattering according to Moliere theory.

=2 Same as 1. Kept for backward compatibility.

= 3 Pure Gaussian scattering according to the Rossi formula.

When traversing ordinary matter, elementary particles undergo deflection from their original trajectory due to the interaction with the atoms. This effect is rather large for charged particles, which are deflected by the electric field of nuclei and electrons via a large number of small elastic collisions. To simulate precisely the transport of particles in matter, it is important to provide a precise description of this effect. Multiple scattering is well described by Moliere theory so we have decided to use IMULS =1 for our simulations.

## Rayleigh scattering

In Rayleigh scattering the interacting  $\gamma$  is not stopped. The variable IRAYL controls this process.

IRAYL =0 (Default) No Rayleigh effect.

=1 Rayleigh effect.

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<sup>v</sup> Seltzer and Berger have calculated the spectra for materials with atomic numbers  $Z = 6, 13, 29, 47, 74, 92$  in the electron (kinetic) energy range 1 keV - 10 GeV. Their tabulated results have been used as input in a multi-parameter-fitting procedure.

In this reaction no secondary particles are generated but the direction of the gamma ray is altered. This effect is not so important above 1 MeV. For now to speed up the simulations we will leave IRAYL = 0. For detail treatment of this problem please see Geant manual.

## Tracking energy thresholds

Lower energy thresholds for both gamma rays and electrons were set at 10 keV. While setting up the geometry and material definitions care was taken in setting materials in such away that gamma ray and electron cross-sections for that material were computed from 10 keV and upwards. The default value for the largest energy considered by Geant is 10 TeV.

## Results

Fig. 6 shows the computed energy deposited spectra for 1.5 MeV incident gamma rays. In the Fig. 6 BGO detector (perfect energy resolution) was used. The BGO crystal was 10 cm X 10 cm X 10 cm in dimension. No attenuator was placed in front of it. In Fig. 6 the escape peak is seen at (1.5 MeV - .511) MeV position. In this figure several X-ray escape peaks along with counts from double Compton events occupy the energy channels between the Compton edge and the photopeak. No double-escape peak is visible. Since there was no material surrounding the detector there is no backscatter peak is visible. The quantity LOG(counts) is plotted on the Y-axis.

Fig. 7 shows two energy deposition spectra for 10 cm X 10 cm X 10 cm NaI detector. The top energy spectrum corresponds to the detector with perfect energy resolution with an air attenuator in the front of the NAI detector. The bottom spectrum corresponds to the detector where parameterized energy resolution was used along with an air attenuator in front of the detector. The incident gamma-energy was 1.5 MeV for these simulations. Each spectra in Fig. 7 show the double-escape peak and the single-escape peak. Several X-ray escape peaks are also visible in the perfect resolution spectra. The bottom plot on the Fig. 7 shows the energy deposition spectra with parameterization for FWHM (as function of energy) from paper by H. V. Nguyen et al.<sup>vi</sup> This parameterization expresses FWHM (keV) = 26.51 E + 4.182 SQRT(E), where E is in MeV. This parameterization gives FWHM of 21 keV at 662 keV and FWHM of 45 keV at 1.5 MeV. The quantity LOG(counts) is plotted on the Y-axis for the plots in Fig. 7.

## Summary

In summary the GEANT package does a reasonable job in simulating the detector response for lower energy gamma rays.

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<sup>vi</sup> “Program in C for parameterizing measured 5” X 5” NaI gamma response functions and unfolding of continuous gamma spectra,” H. V. Nguyen et al., Computer Physics Communications 93 (1996) 303-321

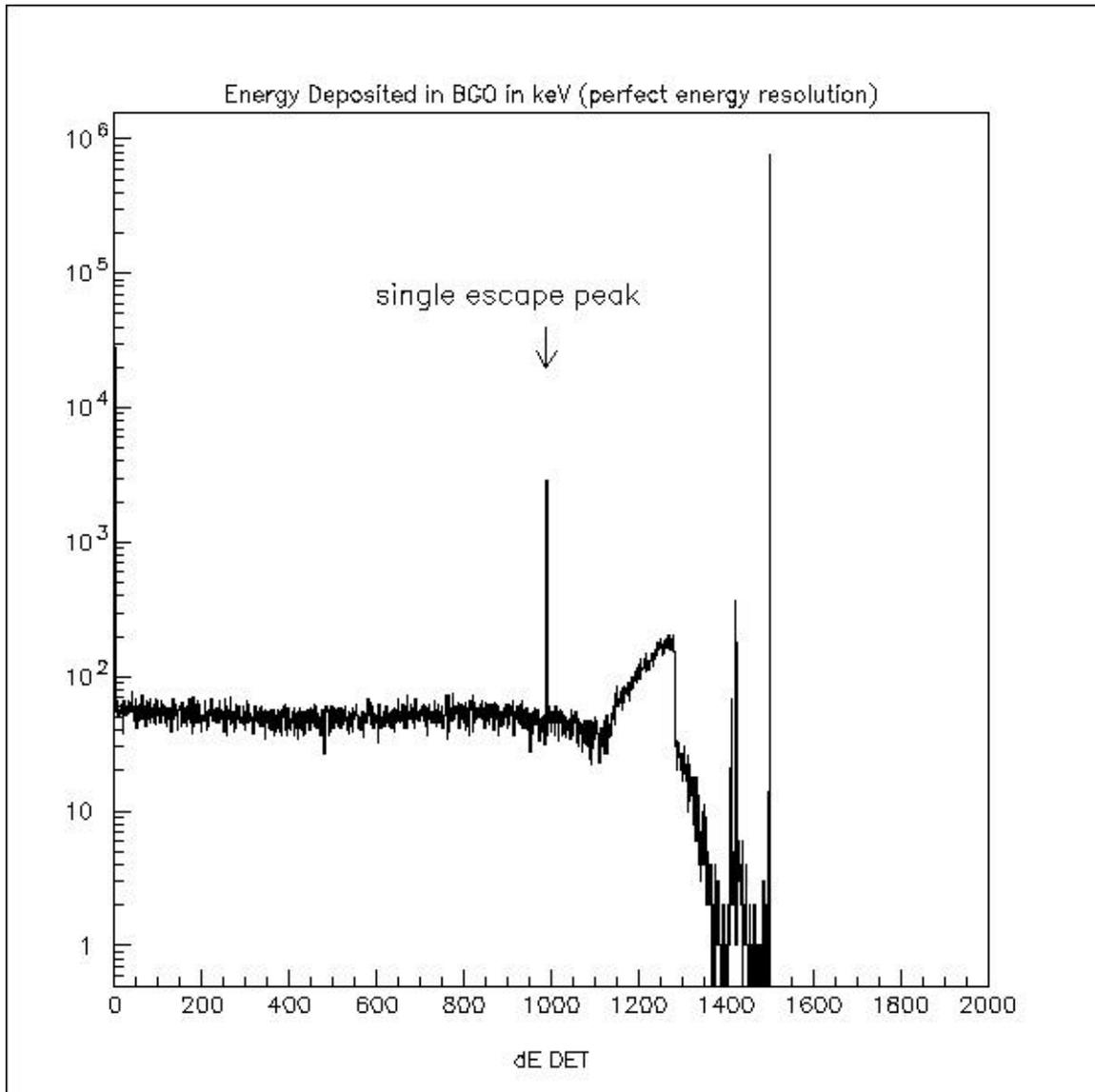


Fig. 6: Energy deposited by 1.5 MeV gamma ray in 10 cm X 10 cm X 10 cm BGO detector with perfect energy resolution.

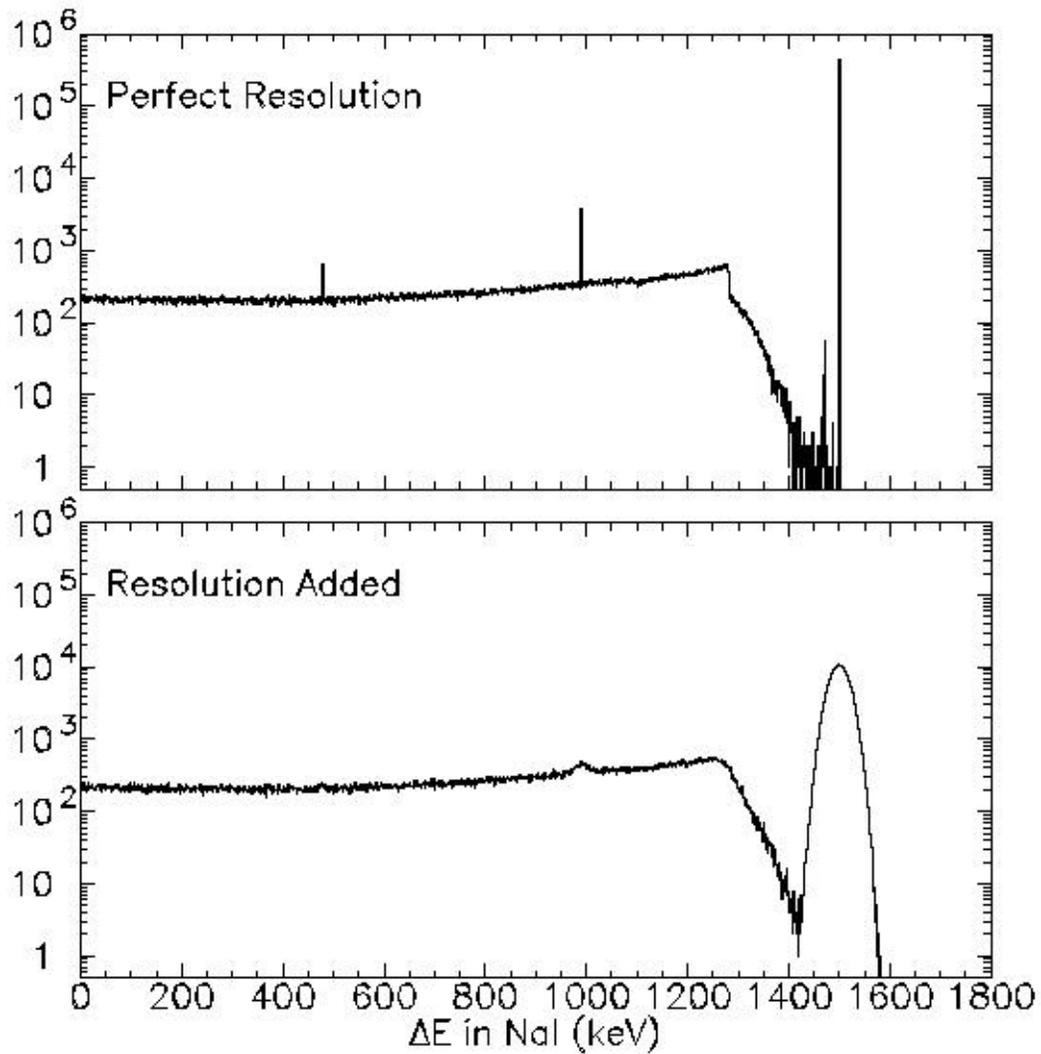


Fig. 7: Energy deposited in 10 cm X 10 cm X 10 cm NaI crystal for 1.5 MeV gamma rays. The top spectrum is for the detector with perfect energy resolution. Energy resolution parameterization was applied while generating the bottom spectra (see text for details).