Lecture notes on Chapter 12: Photon Monte Carlo Simulation

Topics covered

- Basic algorithms of Monte Carlo photon interaction and transport
- Basic, relevant interaction processes, dominance regions
- Flowchart for a photon Monte Carlo code

12.1 Basic photon interaction processes

The photon interaction processes that should be modeled by a photon Monte Carlo code are:

- Pair production in the nuclear field (plus triplet production)
- The Compton interaction (incoherent scattering)
- The photoelectric interaction
- The Rayleigh interaction (coherent scattering)

12.1.1 Pair production in the nuclear field ...

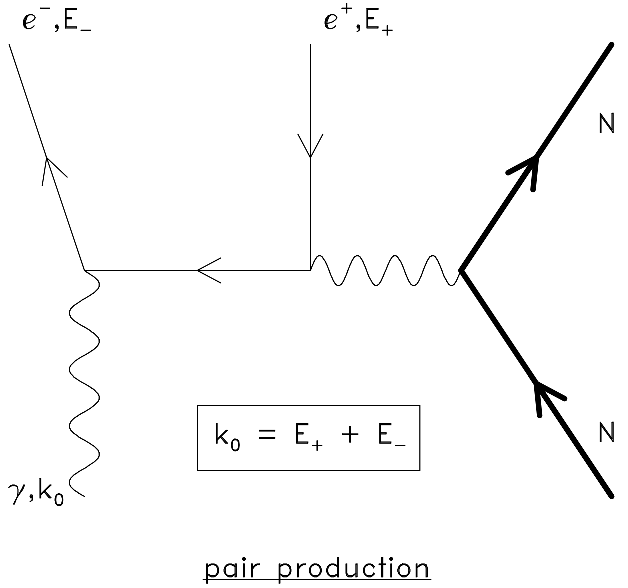

Figure 1: The Feynman diagram depicting pair production in the field of a nucleus. Occasionally (suppressed by a factor of $1/Z$), "triplet" production occurs whereby the incoming photon interacts with one of the electrons in the atomic cloud resulting in a final state with two electrons and one positron. (Picture not shown.)

… 12.1.1 Pair production in the nuclear field …

- A photon can interact in the field of a nucleus, annihilate and produce an electron-positron pair.
- A third body, usually a nucleus, is required to be present to conserve energy and momentum. This interaction scales as Z^2 for different nuclei. Materials containing high atomic number materials more readily convert photons into charged particles than do low atomic number materials.
- Greater than 50 MeV or so in all materials, the pair and bremsstrahlung interactions dominate.

... 12.1.1 Pair production in the nuclear field ...

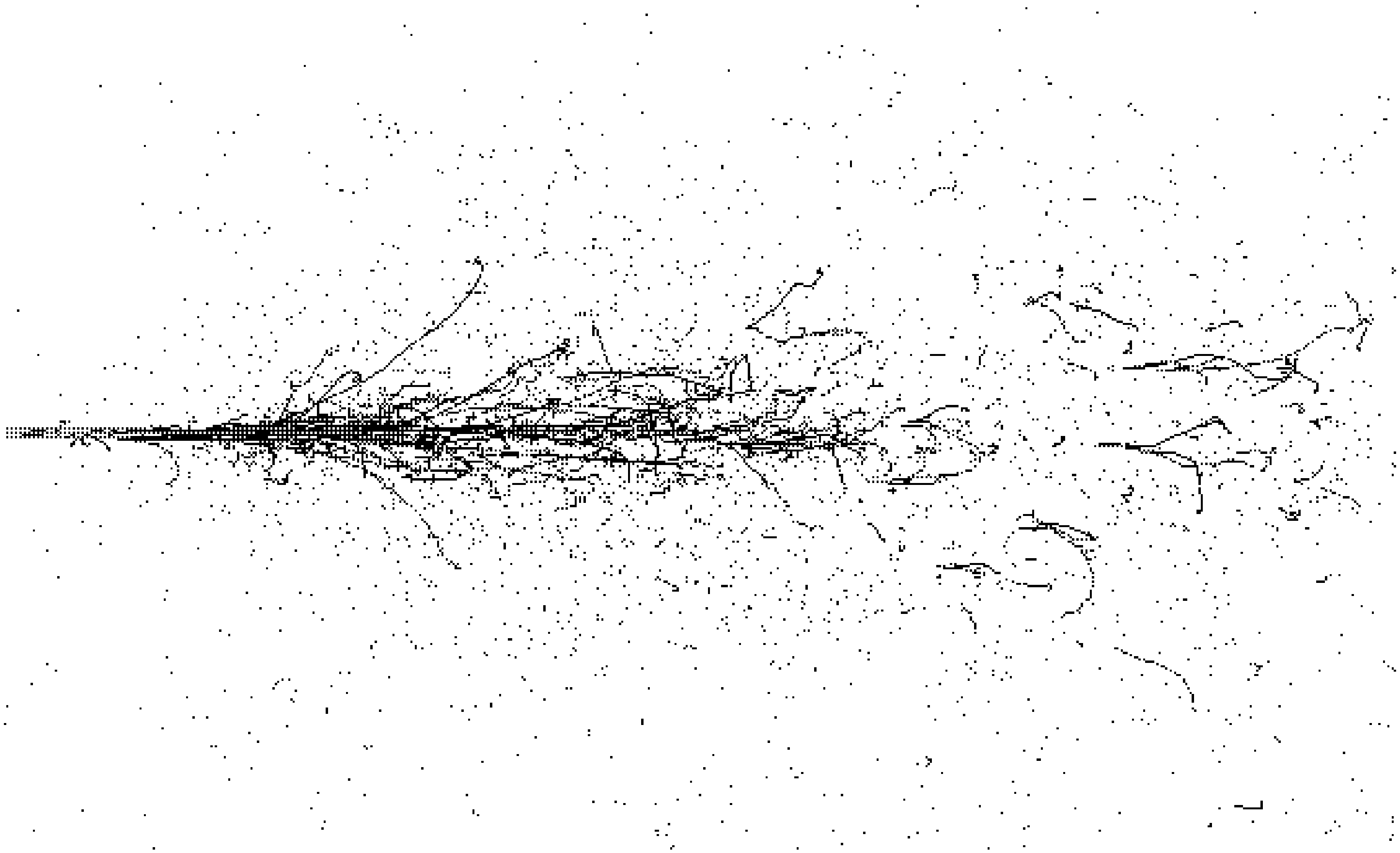

Figure 2: A simulation of the cascade resulting from five 1.0 GeV electrons incident from the left on a target. The electrons produce photons which produce electron-positron pairs and so on until the energy of the particles falls below the cascade region. Electron and positron tracks are shown with black lines. Photon tracks are not shown explaining why some electrons and positrons appear to be “disconnected”. This simulation depicted here was produced by the EGS4 code and the system for viewing the trajectories is called EGS_Windows.

… 12.1.1 Pair production in the nuclear field …

The high-energy limit of the pair production cross section per nucleus takes the form:

$$\lim_{\alpha\to\infty} \sigma_{\rm pp}(\alpha) = \sigma_0^{\rm pp} Z^2 \left(\ln(2\alpha) - \frac{109}{42} \right) \ , \tag{1}$$

where $\alpha = E_\gamma/m_e c^2$, We note that the cross section grows logarithmically with incoming photon energy.

The kinetic energy distribution of the electrons and positrons is remarkably "flat" except near the kinematic extremes of $K_\pm = 0$ and $K_\pm = E_\gamma - 2m_e c^2$. Note as well that the rest-mass energy of the electron-positron pair must be created and so this interaction has a threshold at $E_\gamma = 2m_e c^2$. It is exactly zero below this energy.

... 12.1.1 Pair production (triplet production) ...

Triplet production

Occasionally it is one of the electrons in the atomic cloud surrounding the nucleus that interacts with the incoming photon and provides the necessary third body for momentum and energy conservation.

This interaction channel is suppressed by a factor of about $1/Z$ relative to the nucleus-participating channel as well as additional phase-space and Pauli exclusion differences.

In this case, the atomic electron is ejected with two electrons and one positron emitted. This is called "triplet" production.

It is common to include the effects of triplet production by "scaling up" the two-body reaction channel and ignoring the 3-body kinematics. This is a good approximation for all but the low-Z atoms.

12.1.2 Compton interaction (incoherent scattering) ...

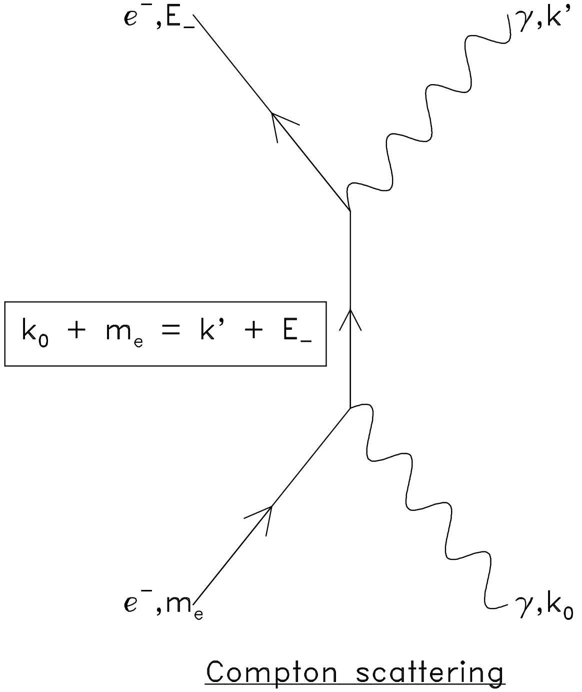

Figure 3: The Feynman diagram depicting the Compton interaction in free space. The photon strikes an electron assumed to be "at rest". The electron is set into motion and the photon recoils with less energy.

12.1.2 … Compton interaction (incoherent scattering) …

The Compton interaction is an inelastic "bounce" of a photon from an electron in the atomic shell of a nucleus. It is also known as "incoherent" scattering in recognition of the fact that the recoil photon is reduced in energy.

At large energies, the Compton interaction approaches asymptotically:

$$\lim_{\alpha \to \infty} \sigma_{\mathrm{inc}}(\alpha) = \sigma_0^{\mathrm{inc}} \frac{Z}{\alpha} \ , \tag{2}$$

where $\sigma_0^{\mathrm{inc}} = 3.33 \times 10^{-25}$ cm^2/nucleus. It is proportional to Z (i.e. the number of electrons) and falls off as $1/E_\gamma$. Thus, the Compton cross section per unit mass is nearly a constant independent of material and the energy-weighted cross section is nearly a constant independent of energy. Unlike the pair production cross section, the Compton cross section decreases with increased energy.

12.1.2 … Compton interaction (incoherent scattering) …

At low energies, the Compton cross section becomes a constant with energy.

$$\lim_{\alpha\to 0} \sigma_{\rm inc}(\alpha) = 2\sigma_0^{\rm inc} Z \ . \tag{3}$$

This is the classical limit and it corresponds to Thomson scattering, which describes the scattering of light from "free" (unbound) electrons.

In almost all applications, the electrons are bound to atoms and this binding has a profound effect on the cross section at low energies. However, above about 100 keV on can consider these bound electrons as "free", and ignore atomic binding effects. This is a good approximation for photon energies down to 100 of keV or so, for most materials. This lower bound is defined by the K-shell energy although the effects can have influence greatly above it, particularly for the low-Z elements.

12.1.2 ... Compton interaction (incoherent scattering) ...

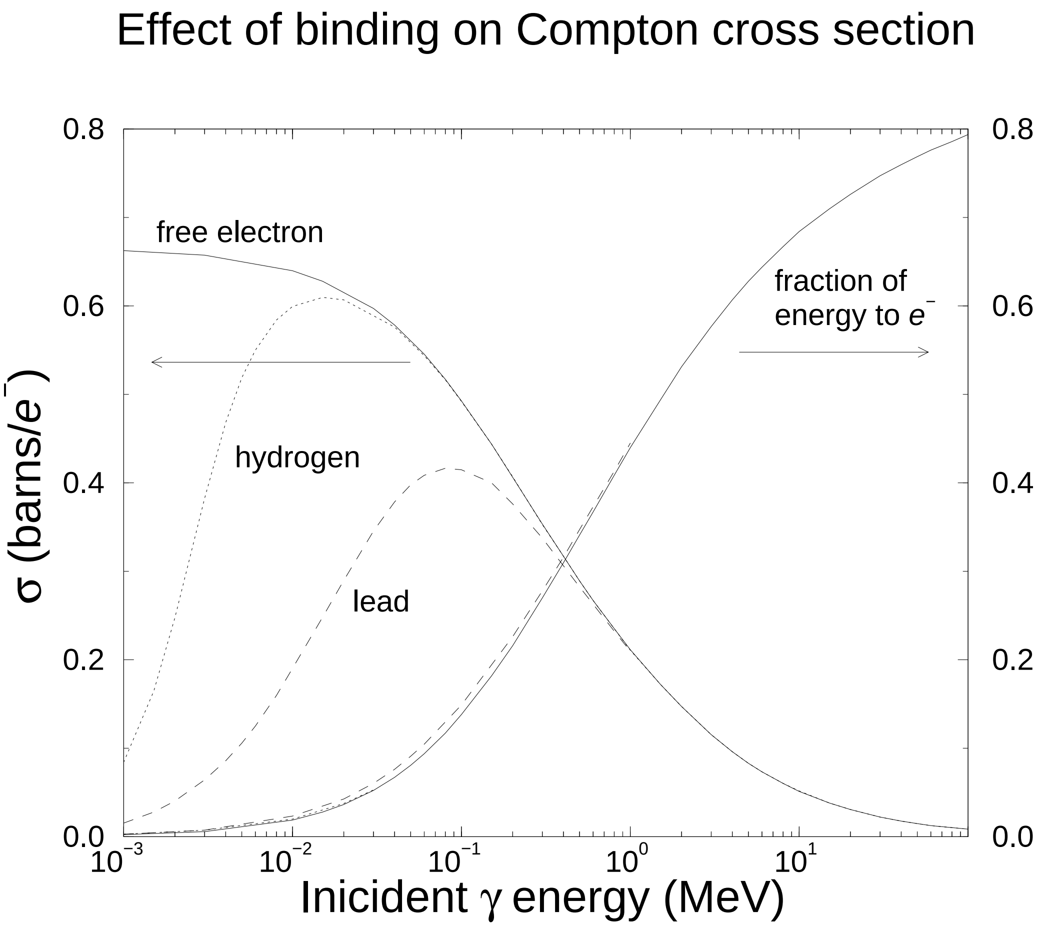

Figure 4: The effect of atomic binding on the Compton cross section.

12.1.2 … Compton interaction (incoherent scattering)

Below this energy the cross section is depressed since the K-shell electrons are too tightly bound to be liberated by the incoming photon. The unbound Compton differential cross section is taken from the Klein-Nishina cross section, derived in lowest order Quantum Electrodynamics, without any further approximation.

It is possible to improve the modeling of the Compton interaction. Namito and Hirayama have considered the effect of binding for the Compton effect as well as allowing for the transport of polarized photons for both the Compton and Rayleigh interactions.

12.1.3 Photoelectric interaction ...

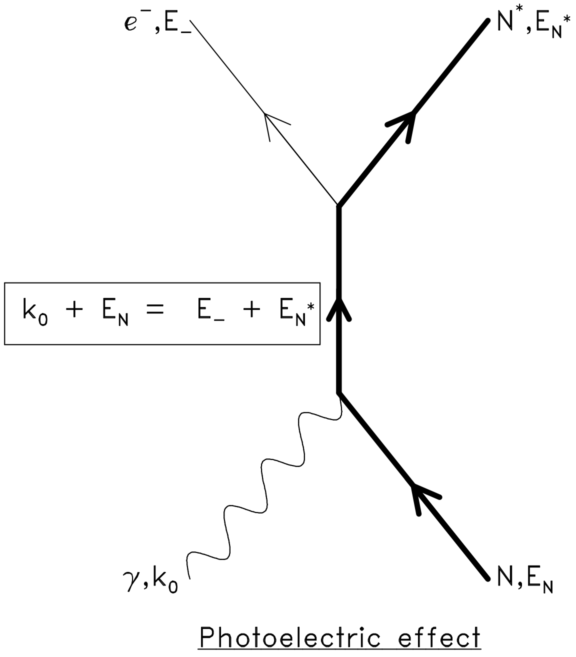

Figure 5: Photoelectric effect

12.1.3 ... Photoelectric interaction ...

The dominant low energy photon process is the photoelectric effect. In this case the photon gets absorbed by an electron of an atom resulting in escape of the electron from the atom and accompanying small energy photons as the electron cloud of the atom settles into its ground state. The theory concerning this phenomenon is not complete and exceedingly complicated. The cross section formulae are usually in the form of numerical fits and take the form:

$$\sigma_{\mathrm{ph}}(E_\gamma) \propto \frac{Z^m}{E_\gamma^n} \; , \tag{4}$$

where the exponent on Z ranges from 4 (low energy, below 100 keV) to 4.6 (high energy, above 500 keV) and the exponent on E_γ ranges from 3 (low energy, below 100 keV) to 1 (high energy, above 500 keV). Note that the high-energy fall-off is the same as the Compton interaction. However, the high-energy photoelectric cross section is depressed by a factor of about $Z^{3.6}10^{-8}$ relative to the Compton cross section and so is negligible in comparison to the Compton cross section at high energies.

12.1.3 … Photoelectric interaction

A useful approximation that applies in the regime where the photoelectric effect is dominant is:

$$\sigma_{\rm ph}(E_\gamma) \propto \frac{Z^4}{E_\gamma^3} \ , \tag{5}$$

which is often employed for simple analytic calculations. However, most Monte Carlo codes employ a table look-up for the photoelectric interaction.

Angular distributions of the photoelectron can be determined according to the theory of Sauter. Although Sauter's theory is relativistic, it appears to work in the non-relativistic regime as well.

12.1.4 Rayleigh (coherent) interaction ...

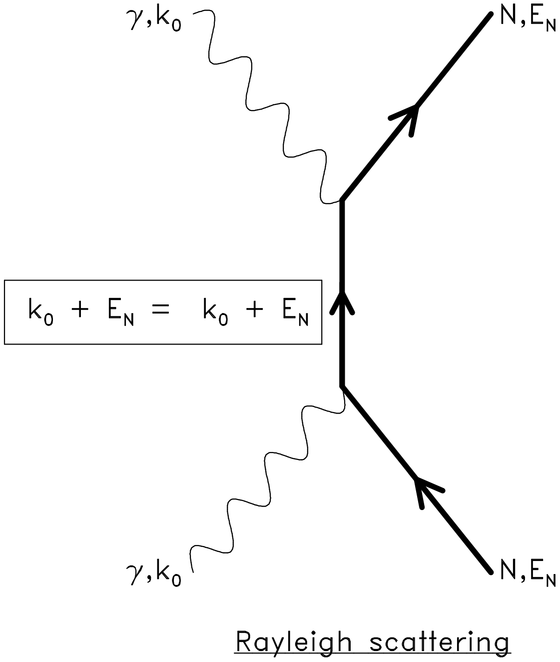

Figure 6: Rayleigh scattering

12.1.4 ...Rayleigh (coherent) interaction...

Now we consider the Rayleigh interaction, also known as coherent scattering.

The Rayleigh cross section is at least an order of magnitude less that the photoelectric cross section. However, it is still important! As can be seen from the Feynman diagram above, the distinguishing feature of this interaction, in contrast to the photoelectric interaction, is that there is a photon in the final state.

If low energy photons impinge on an optically thick shield both Compton and Rayleigh scattered photons will emerge from the far side. Moreover, the proportions will be a sensitive function of the incoming energy.

The coherent interaction is an elastic (no energy loss) scattering from atoms. It is not good enough to treat molecules as if they are made up of independent atoms. A good demonstration of the importance of molecular structure was demonstrated by Johns and Yaffe.

12.1.4 ...Rayleigh (coherent) interaction

The Rayleigh differential cross section has the following form:

$$\sigma_{\mathrm{coh}}(E_\gamma, \Theta) = \frac{r_e^2}{2}(1 + \cos^2\Theta)[F(q, Z)]^2 \ , \tag{6}$$

where
r_e is the classical electron radius (2.8179×10^{-13} cm),
q is the momentum-transfer parameter, $q = (E_\gamma/hc)\sin(\Theta/2)$, and
$F(q, Z)$ is the atomic form factor.

$F(q, Z)$ approaches Z as q goes to zero either by virtue of E_γ going to zero or Θ going to zero. The atomic form factor also falls off rapidly with angle although the Z-dependence increases with angle to approximately $Z^{3/2}$.

The tabulation of the form factors published by Hubbell and Øverbø.

12.1.4 Relative importance of various processes ...

We now consider the relative importance of the various processes involved.

For carbon, a moderately low-Z material, the relative strengths of the photon interactions versus energy is shown below. For this material we note three distinct regions of single interaction dominance:
photoelectric below 20 keV,
pair above 30 MeV and
Compton in between.

The almost order of magnitude depression of the Rayleigh and triplet contributions is some justification for the relatively crude approximations we have discussed. For lead, shown below, there are several differences and many similarities.

12.1.4 ... Relative importance of various processes ...

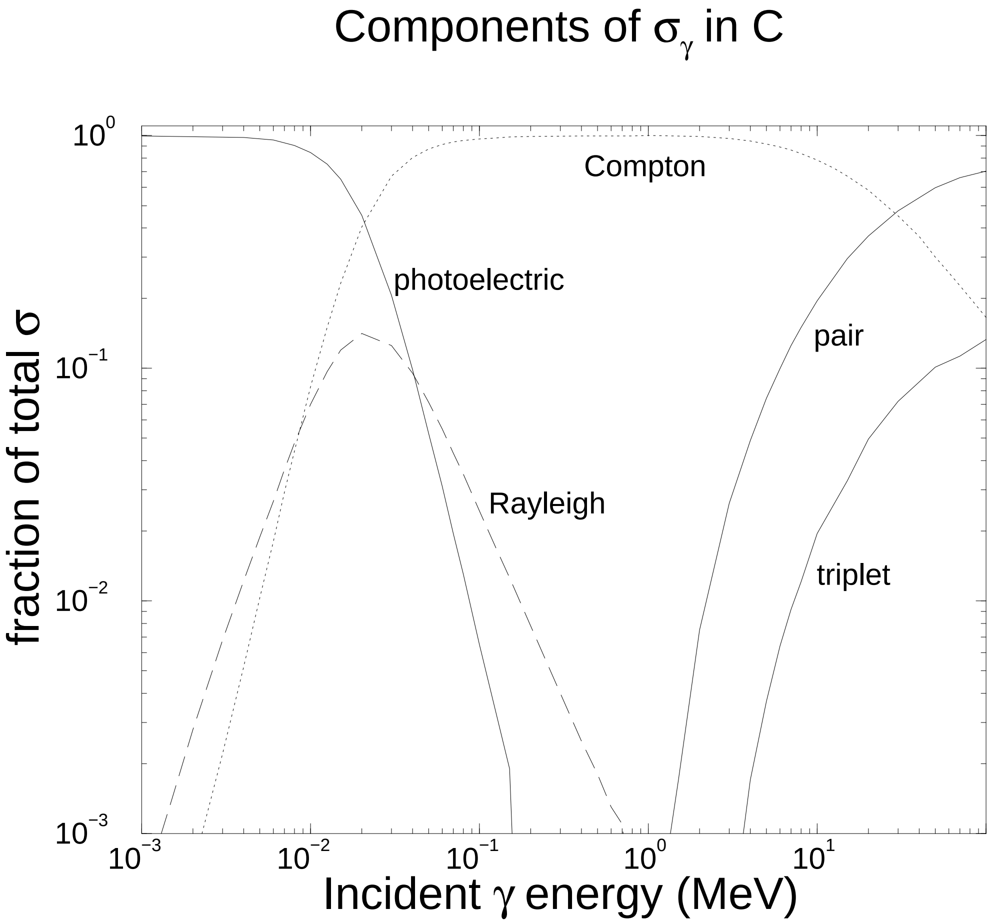

Figure 7: Components of the photon cross section in Carbon.

12.1.4 ... Relative importance of various processes ...

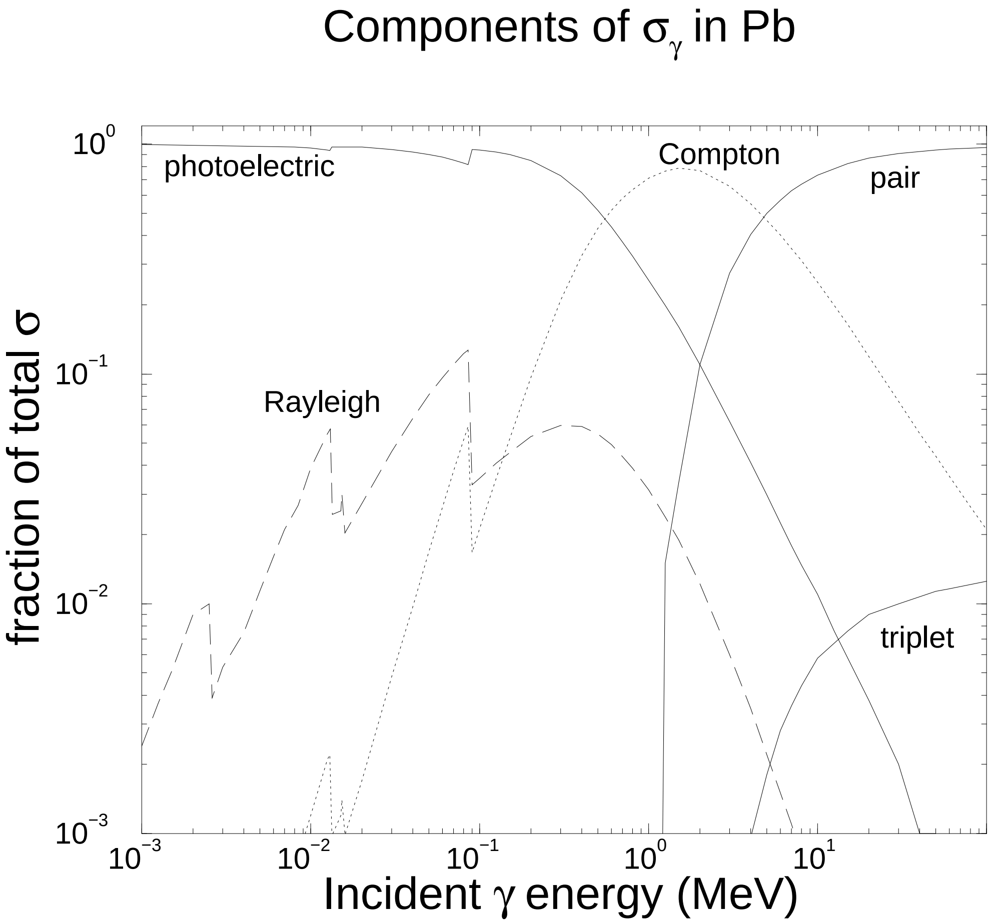

Figure 8: Components of the photon cross section in Lead.

12.1.4 ... Relative importance of various processes ...

The same comment about the relative unimportance of the Rayleigh and triplet cross sections applies for lead.

The "Compton dominance" section is much smaller, now extending only from 700 keV to 4 MeV.

We also note quite a complicated structure below about 90 keV, the K-shell binding energy of the lead atom. Below this threshold, atomic structure effects become very important.

Finally, we consider the total cross section versus energy for the materials hydrogen, water and lead, shown in Figure 9.

12.1.4 ... Relative importance of various processes ...

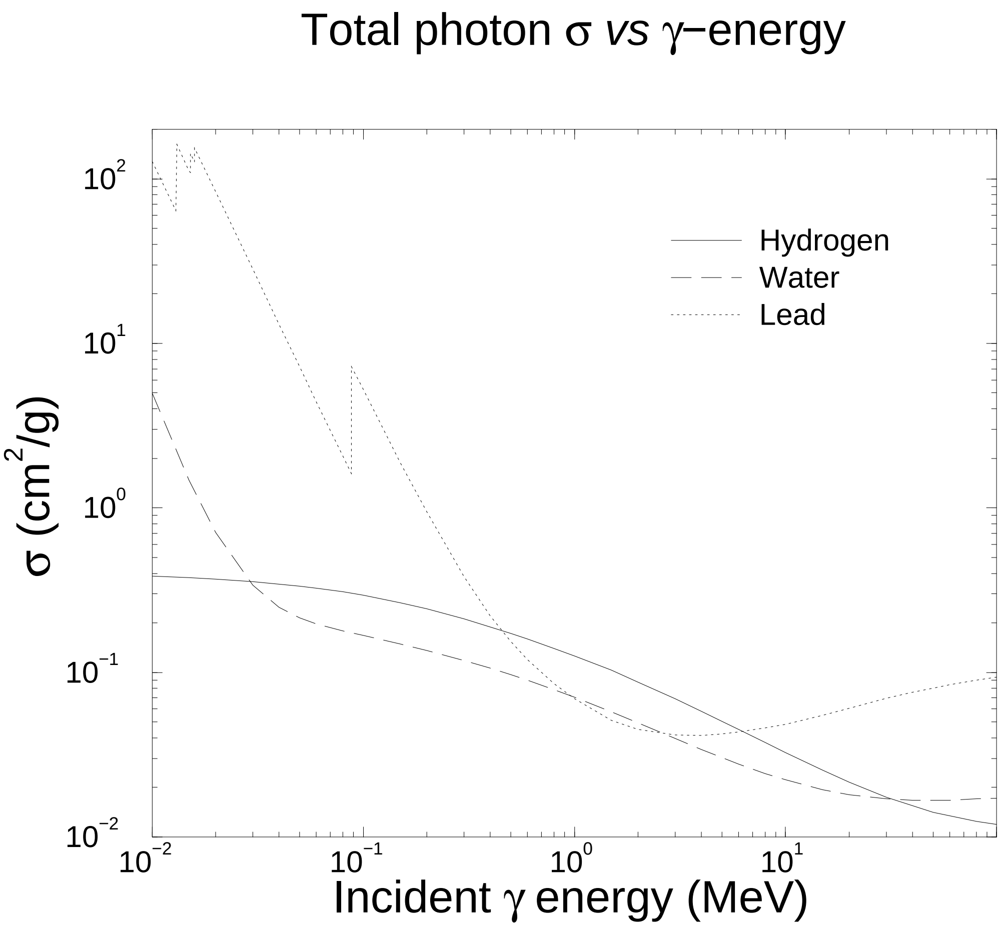

Figure 9: Total photon cross section vs. photon energy.

12.1.4 ... Relative importance of various processes ...

The total cross section is plotted in the units cm^2/g.

The Compton dominance regions are equivalent except for a relative $\overline{A/Z}$ factor.

At high energy the Z^2 dependence of pair production is evident in the lead.

At lower energies the $Z^n (n > 4)$ dependence of the photoelectric cross section is quite evident.

12.2 Photon transport logic ...

We now discuss a simplified version of photon transport logic. It is simplified by ignoring electron creation and considering that the transport occurs in only a single volume element and a single medium.

This photon transport logic is schematized in the figure below.

An initial photon's parameters are present at the top of an structure that we shall name `STACK`.

This structure retains particle phase space characteristics for processing.

A transport cutoff is defined. A photons whose energy falls below this cutoff is is considered to be absorbed "on the spot". (Removed from the `STACK`.)

We consider that they do not contribute significantly to any tallies of interest and can be ignored. Physically, this step is not really necessary—it is only a time-saving maneuver. In "real life" low-energy photons are absorbed by the photoelectric process and vanish. (This is, actually, a bit of a fiction. Energetic discussion to ensue.)

12.3 ... Photon transport logic ...

The logic flow of photon transport proceeds as follows.

A source function places an initial photon on the `STACK`, defining its energy, direction and position vector, starting region number, and “weight”.
(A particle’s weight is usually assigned to unity, but may have other values based on variance reduction methods, covered in a later chapter.

The photon transport function, described in the following figure, first tests to see if the energy is below the transport cutoff. If it is below the cutoff, the history is terminated. If the `STACK` is empty then a new particle history is started.

If the energy is above the cutoff, then the distance to the next interaction site is chosen, following the discussion in Chapter 8, Transport in media, interaction models.

12.4 ... Photon transport logic ...

The photon is then transported, that is transported to the point of interaction. (If the geometry is more complicated than just one region, transport through different elements of the geometry would be taken care of here.)

If the photon, by virtue of its transport, has left the volume defining the problem then it is discarded.

Otherwise, the branching distribution is sampled to see which interaction occurs. Having done this, the surviving particles (new ones may be created, some disappear, the characteristics of the initial one will almost certainly change) have their energies, directions and other characteristics chosen from the appropriate distributions.

The surviving particles are put on the `STACK`.

Lowest energy ones should be put on the top of the `STACK` to keep the size of the `STACK` as small as possible.

Then the whole process takes place again until the `STACK` is empty and all the incident particles are used up.

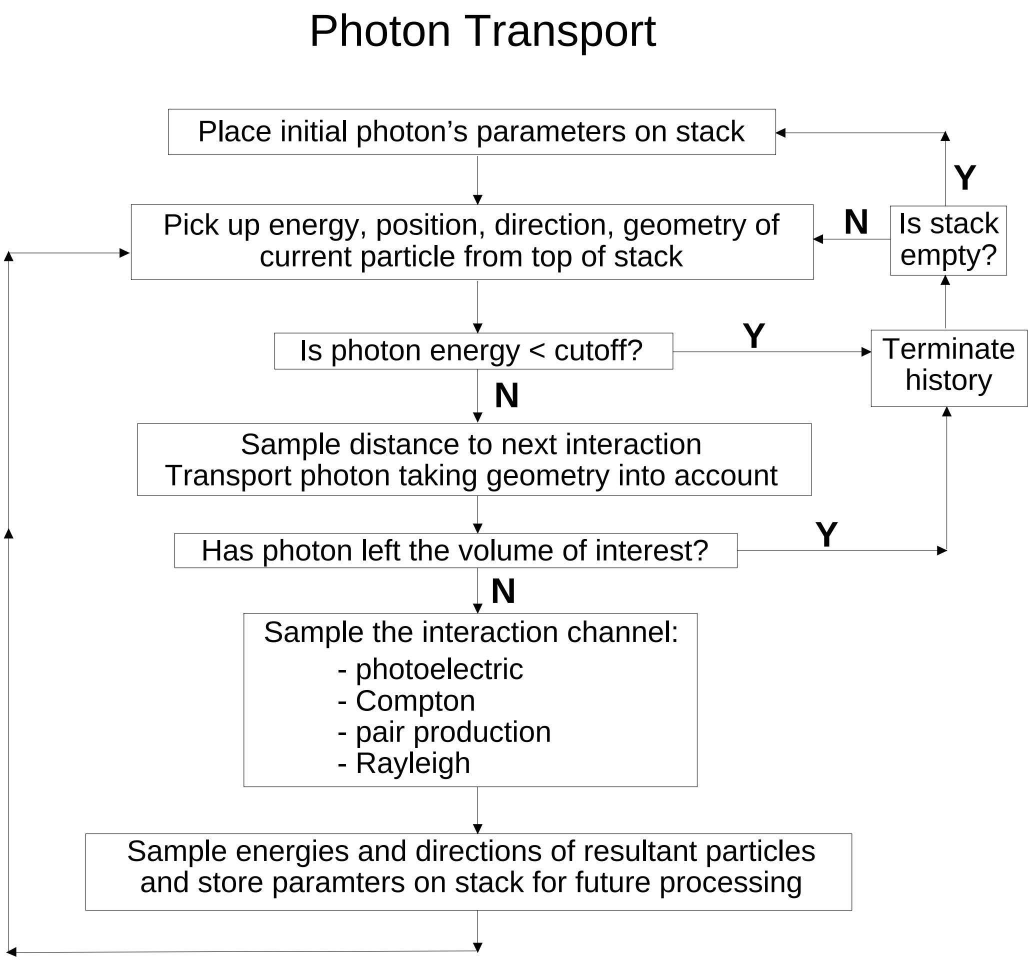

Figure 10: "Bare-bones" photon transport logic.