Lecture notes:
Photon Monte Carlo simulation

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"I could have done it in a much more complicated way"
said the red Queen, immensely proud.
Lewis Carroll

1 Introduction

In this lecture we discuss the basic mechanism by which the simulation of photon interaction and transport is undertaken in the EGS4 code. We start with a review of the basic interaction processes that are involved, the approximations made by EGS4, some recent improvements and their relative importance. We discuss when and how one goes about choosing, by random selection, which process occurs. We discuss the rudimentary geometry involved in the transport and deflection of photons. We conclude with a schematic presentation of the logic flow executed by EGS4 in implementing all this physics. Except for the discussion of recent improvements, this discussion is a condensation of the material in the EGS4 manual [1] which should be consider co-requisite reading for those interested in the fine details.

2 Basic photon interaction processes

We now give a brief discussion of the photon interaction processes modeled by EGS4.

2.0.1 Pair production

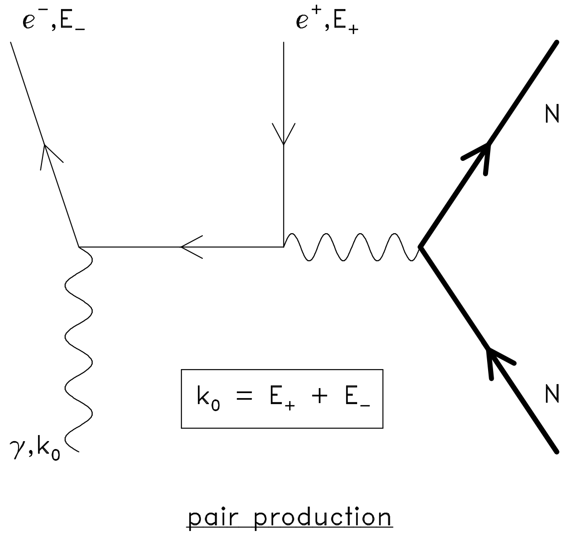

Figure 1: Pair production in the field of an atom. Occasionally (suppressed by a factor of $1/Z$), "triplet" production occurs whereby the incoming photon interacts with one of the electrons in the atomic cloud resulting in a final state with two electrons and one positron.

As seen in fig. 1, a photon can interact in the field of a nucleus, annihilate and produce a electron-positron pair. This interaction scales as Z^2 for different nuclei. Occasionally (suppressed by a factor of $1/Z$) it is one of the electrons in the atomic cloud that interacts with the incoming photon. In this case, the atomic electron can be ejected with two electrons and one positron emitted. This is called "triplet" production. The effects of triplet production are included in the total cross section although EGS4 only produces pairs. This is a good approximation for all but the low-Z atoms.

Atomic electron screening is included in the EGS4 calculation of the pair production cross sections. Below 50 MeV EGS4 employs data from a compilation by Storm and Israel [2]. Above 50 MeV an extreme relativistic formalism is employed along with Coulomb corrections. The formulae for these processes are quite lengthy and sampling these interactions is quite involved. The interested reader is encouraged to consult Section 2.7 of the manual SLAC-265 [1] for more details on how the pair production cross section is sampled and what further approximations are made.

In its default configuration the newly-created e^+e^- particles are projected at a fixed angle relative to the initial γ's direction. This angle is $\Theta = m_0c^2/E_\gamma$, where m_0c^2 is the electron rest-mass energy. Recently this situation has been improved by incorporating a realistic angular distribution [3].

2.0.2 Compton interaction

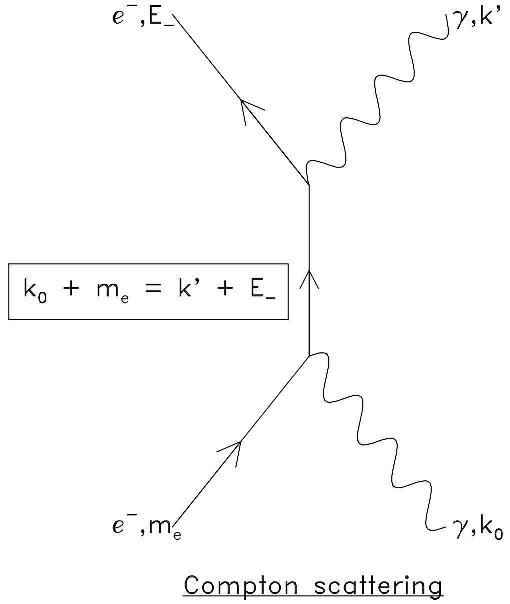

Figure 2: Compton interaction in free space.

The Compton interaction is an inelastic "bounce" of a photon from an electron in the atomic shell of a nucleus. EGS4 treats these bound electrons as "free", ignoring atomic binding effects. As seen in fig. 3, this is a good approximation for photon energies down to 10's of keV, 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. 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 Compton interaction scales as Z for different atoms. The differential cross section is taken from the Klein-Nishina cross section, derived in lowest order Quantum Electrodynamics, without any further approximation.

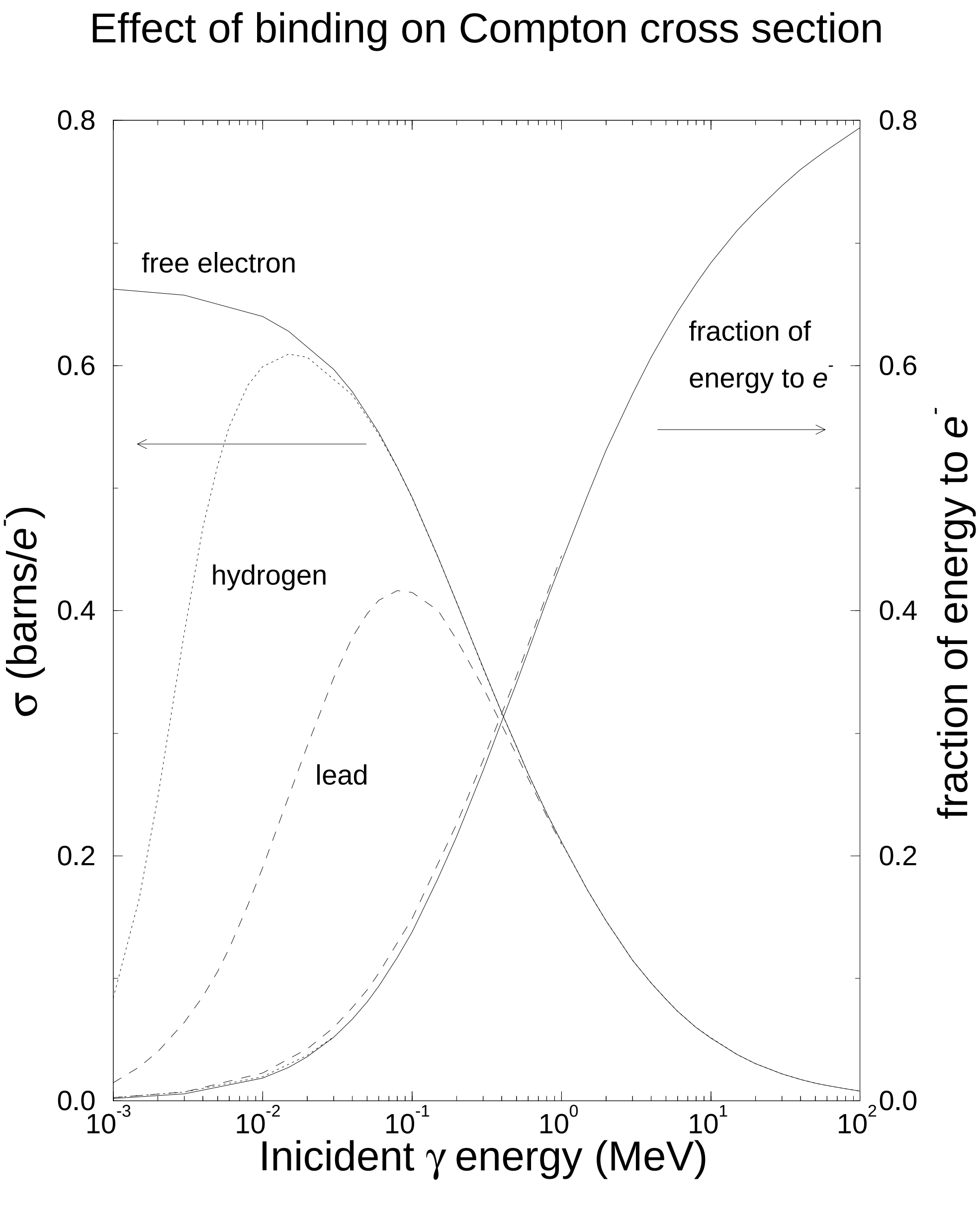

Figure 3: Effect of binding on the Compton cross section.

Recent improvements to the Comptom modeling have been accomplished by Namito *et al.*[1] who included the effect of binding for the Compton effect as well as allowing for the transport of polarised photons for both the Compton and Rayleigh interactions.

2.0.3 Photoelectric interaction

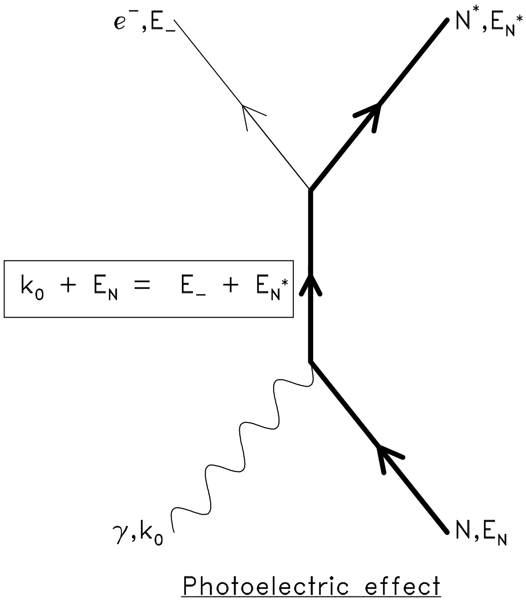

Figure 4: Photoelectric effect

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. It scales as $Z^4 \to Z^5$, depending on the photon energy.

Those interested in low energy applications should be made aware of the approximations made by EGS4. The photoelectron is ejected in the same direction as the incoming photon. Realistic electron angular distributions have been included [4] and are distributed with the unix and PC versions of the code. The standard EGS4 version also does not set the fluorescent photons in motion. Advanced EGS4 users can make use of code that creates and transports K_α and K_β photons. This code is distributed with all EGS4 distributions. Again, the interested reader is referred to the EGS4 manual for details.

2.0.4 Rayleigh (coherent) interaction

A somewhat less important low energy process is Rayleigh, or coherent, scattering. This can be viewed as elastic (no energy loss) scattering from atoms. EGS4 treats all atoms as if they contribute independently to coherent scattering, not a terribly good approximation. Rayleigh scattering varies in a complicated way with different atoms, like Z^2 for small scattering angles and Z^3 for large scattering angles.

[1]Those seeking more information on these improvements should contact the author, Dr. Yoshihito Namito, National Laboratory for High Energy Physics, Oho, Tsukuba-shi, Ibaraki-ken, 305, Japan, e-mail: QV04@kekcc.kek.jp

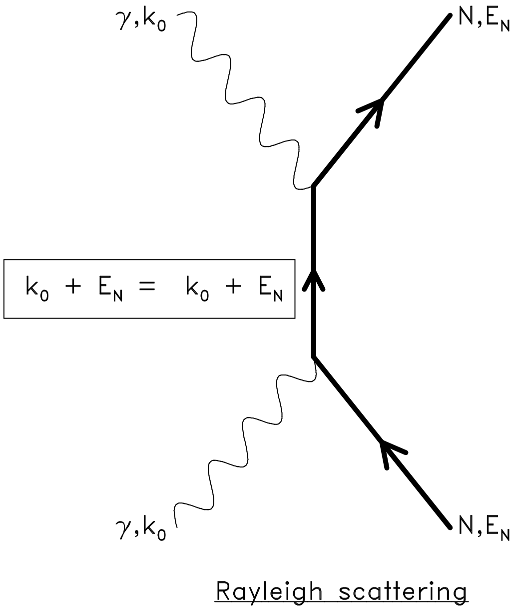

Figure 5: Rayleigh scattering

2.1 Relative importance of various processes

We now consider the relative importance of the various processes involved, from a pedagogical point of view and as a means of justifying some of the approximations made in EGS4.

For carbon, a moderately low-Z material, the relative strengths of the photon interactions versus energy is shown in fig. 6. 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 in fig. 7, there are several differences and many similarities. The same comment about the relative unimportance of the Rayleigh and triplet cross sections applies. 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 fig. 8. 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.

3 Simple sampling

Imagine that we are in an infinite medium and we wish to transport a photon in it. We know that this medium interacts with the photon the strength of which is expressed by the cross section, in units L^{-1}. The probability that the photon has not interacted after being transported a distance t, is given by:

$$p(t) = \Sigma e^{-\Sigma t}, \tag{1}$$

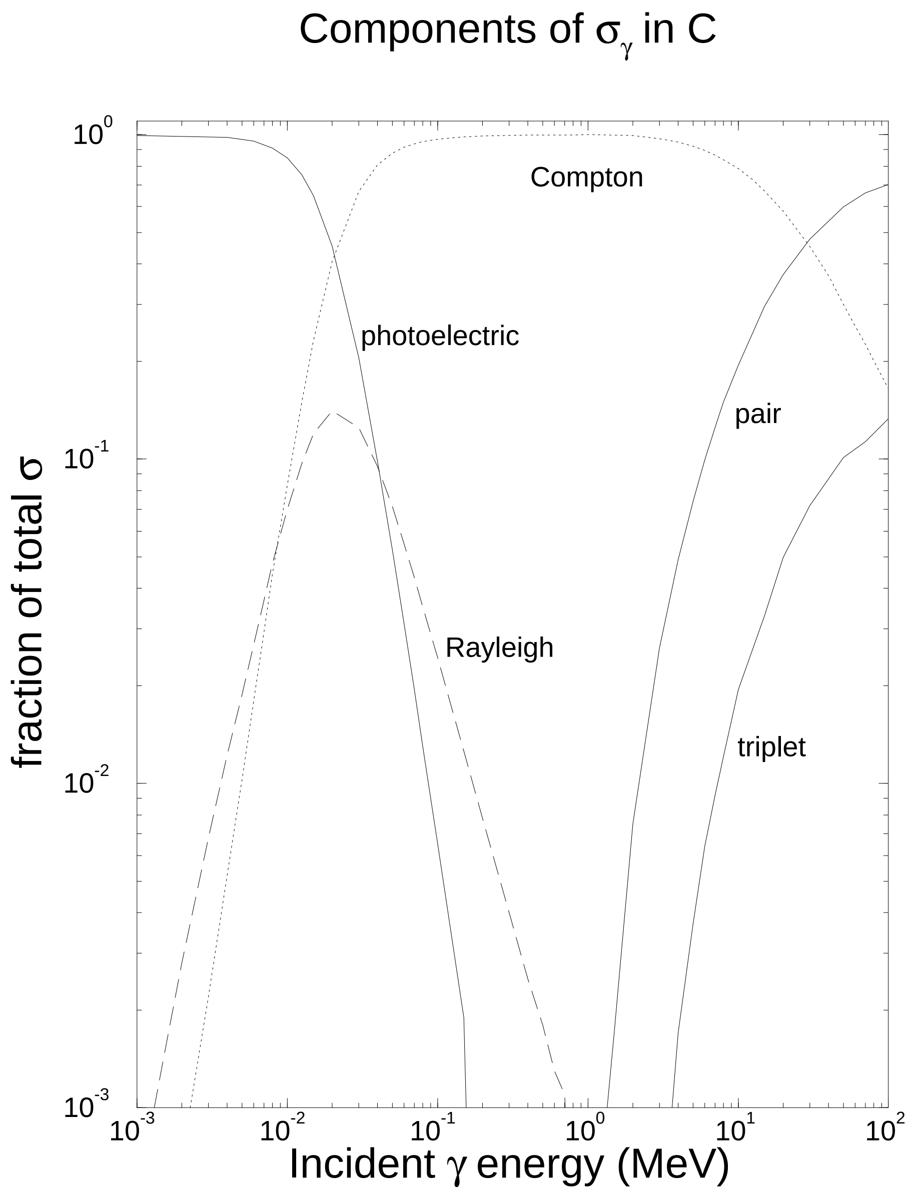

Figure 6: Components of the photon cross section in Carbon.

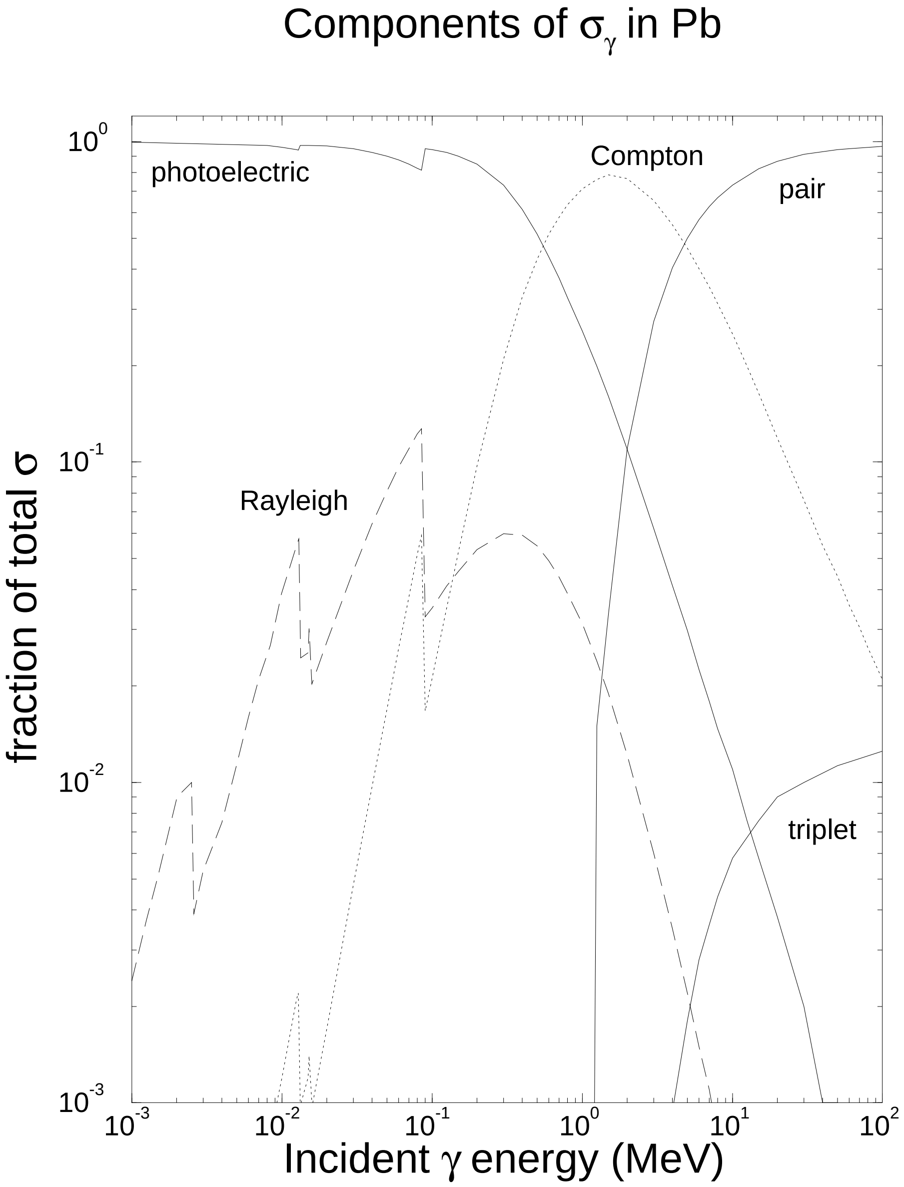

Figure 7: Components of the photon cross section in Lead.

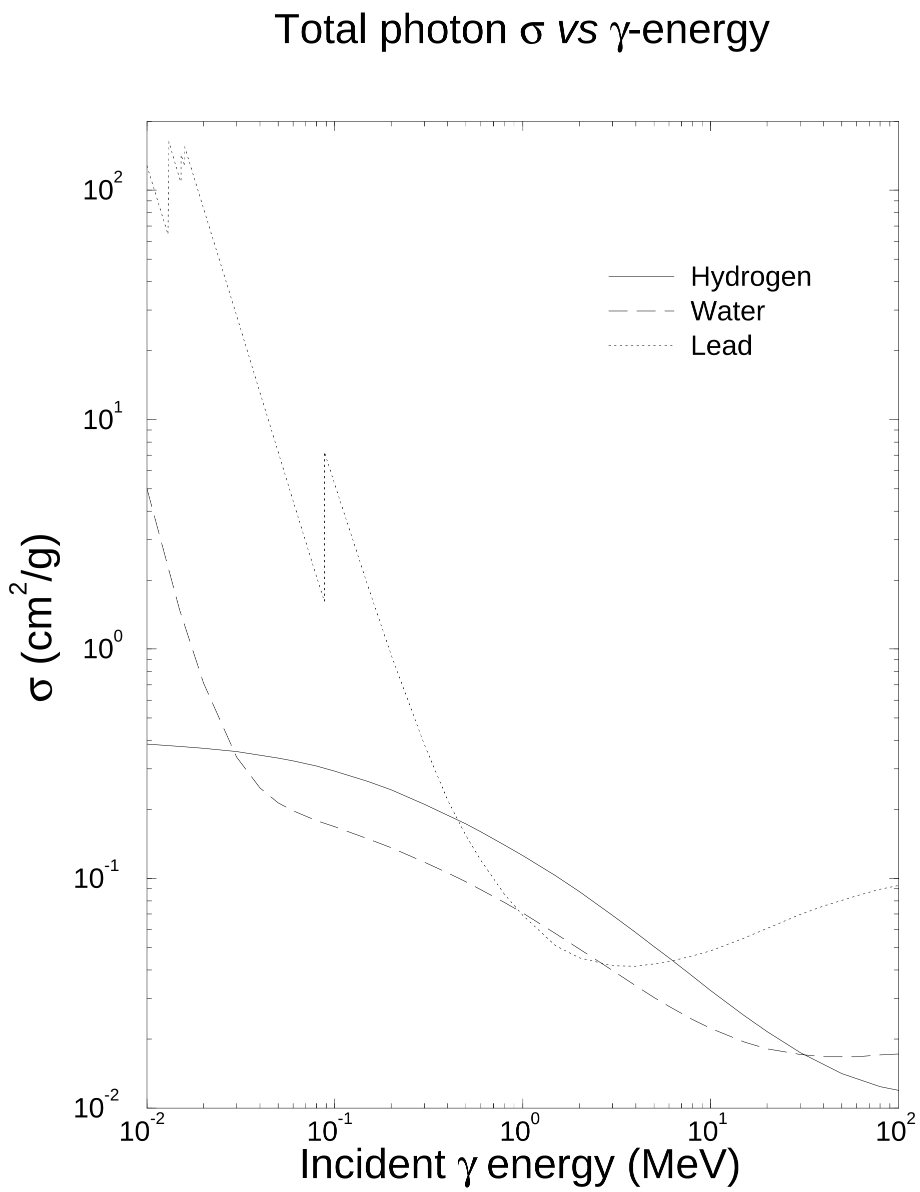

Figure 8: Total photon cross section *vs.* photon energy.

the well known exponential attenuation law. How then, do we decide the distance to the interaction that must occur eventually?

The answer is given by one of the simplest but most relevant examples of the "direct sampling" method. We shall discuss this method in detail in a later lecture but we will work through this example quickly, in "cook book" fashion.

1. Construct the cumulative distribution function (CDF):

$$c(t) = \int_0^t \mathrm{d}t' \Sigma e^{-\Sigma t'} = 1 - e^{-\Sigma t}. \tag{2}$$

   (It is important that $p(t)$ be properly normalised so that $c(\infty) = 1$.)

2. Construct the inverse of CDF,

$$t = -\frac{1}{\Sigma}\log[1 - c(t)]. \tag{3}$$

3. Let ξ be a random number uniformly distributed so that $0 < \xi < 1$. Then, the distance of the next interaction is:

$$t = -\frac{1}{\Sigma}\log(1 - \xi). \tag{4}$$

4. Trick. If ξ is uniformly distributed between 0 and 1, then so is $1 - \xi$. So, to save computer time, rewrite as,

$$t = -\frac{1}{\Sigma}\log(\xi). \tag{5}$$

   Warning. You must trap for the case $\xi = 0$!

5. Σ is the total cross section including all interactions. If more than one interaction comprises Σ, then another random number must be selected to choose which interaction occurs. For example, if we know there was a 90% chance of a photoelectric interaction and 10% of a Rayleigh scattering, select another random number. If $\xi < 0.9$, it is a photoelectric event, otherwise it is a Rayleigh scattering.

6. Simulate the interaction, deduct energy, change direction, create new particles, *etc.* We shall see soon how this all fits together in a realistic photon transport algorithm.

3.1 Geometrical transport

Transport and deflection are carried out using some very simple geometrical constructs. Given that a photon has position $\vec{x}$, direction $\vec{u}$ and distance to travel s, the new position, $\vec{x}'$, is given by:

$$\vec{x}' = \vec{x} + \vec{u}s, \tag{6}$$

or

$$\begin{aligned} x' &= x + us \\ y' &= y + vs \\ z' &= z + ws \end{aligned} \tag{7}$$

where $\vec{x} = (x, y, z)$, $\vec{x'} = (x', y', z')$, and $\vec{u} = (u, v, w) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The angles θ and ϕ are defined with respect to the z-axis of the problem.

If after a given path-length an interaction takes place, generally the direction of the particle will have to be changed. The equations that describe the directions of a particle before and after scattering are derived as follows: Given scattering angles Θ and Φ, a particle going along the z-axis [direction $(0,0,1)$] is deflected into the direction $(\sin\Theta\cos\Phi, \sin\Theta\sin\Phi, \cos\Theta)$. The rotation for an arbitrary incident direction (u,v,w) is accomplished by means of the rotation matrix:

$$\Re = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{8}$$

and the new direction cosines and new angles are given by:

$$\begin{aligned} u' = \sin\theta'\cos\phi' &= u\cos\Theta + \sin\Theta(w\cos\Phi\cos\phi - \sin\Phi\sin\phi) \\ v' = \sin\theta'\sin\phi' &= v\cos\Theta + \sin\Theta(w\cos\Phi\sin\phi + \sin\Phi\cos\phi) \\ w' = \cos\theta' &= w\cos\Theta - \sin\Theta(\sin\theta\cos\Phi) \end{aligned} \tag{9}$$

4 Photon transport logic

We now discuss a simplified version of the photon transport logic in EGS4. 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 schematised in fig. 9. Imagine that an initial photon's parameters are present at the top of the `STACK`. (The `STACK` is an array that retains particle characteristics for processing.) The characteristics are picked up and the energy tested to see if it 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 the previous section. The photon is then transported. (If the geometry was 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 are put on the top of the `STACK` to prevent `STACK` overflow. Then the whole process takes place again until the `STACK` is empty and all the incident particles are used up.

This is a "bare-bones" version of the EGS4 photon transport routine. The user is encouraged to examine the `PHOTON` (the name of the EGS4 photon transport subroutine) flow chart given in the EGS4 manual.

References

[1] W.R. Nelson, H. Hirayama and D.W.O. Rogers, *The EGS4 Code System*, Stanford Linear Accelerator Center Report SLAC-265 (Stanford Calif) (1985).

[2] E. Storm and H. I. Israel, *Photon Cross Sections from 1 keV to 100 MeV for Elements Z=1 to Z=100*, Atomic Data and Nuclear Data Tables 565 (1970).

[3] A.F. Bielajew, *Improved angular sampling for pair production in the EGS4 code system*, NRCC Report: PIRS-0287 (1991).

[4] A.F. Bielajew and D.W.O. Rogers, *Photoelectron angular distribution in the EGS4 code system*, National Research Council of Canada Report PIRS-0058 (1986).

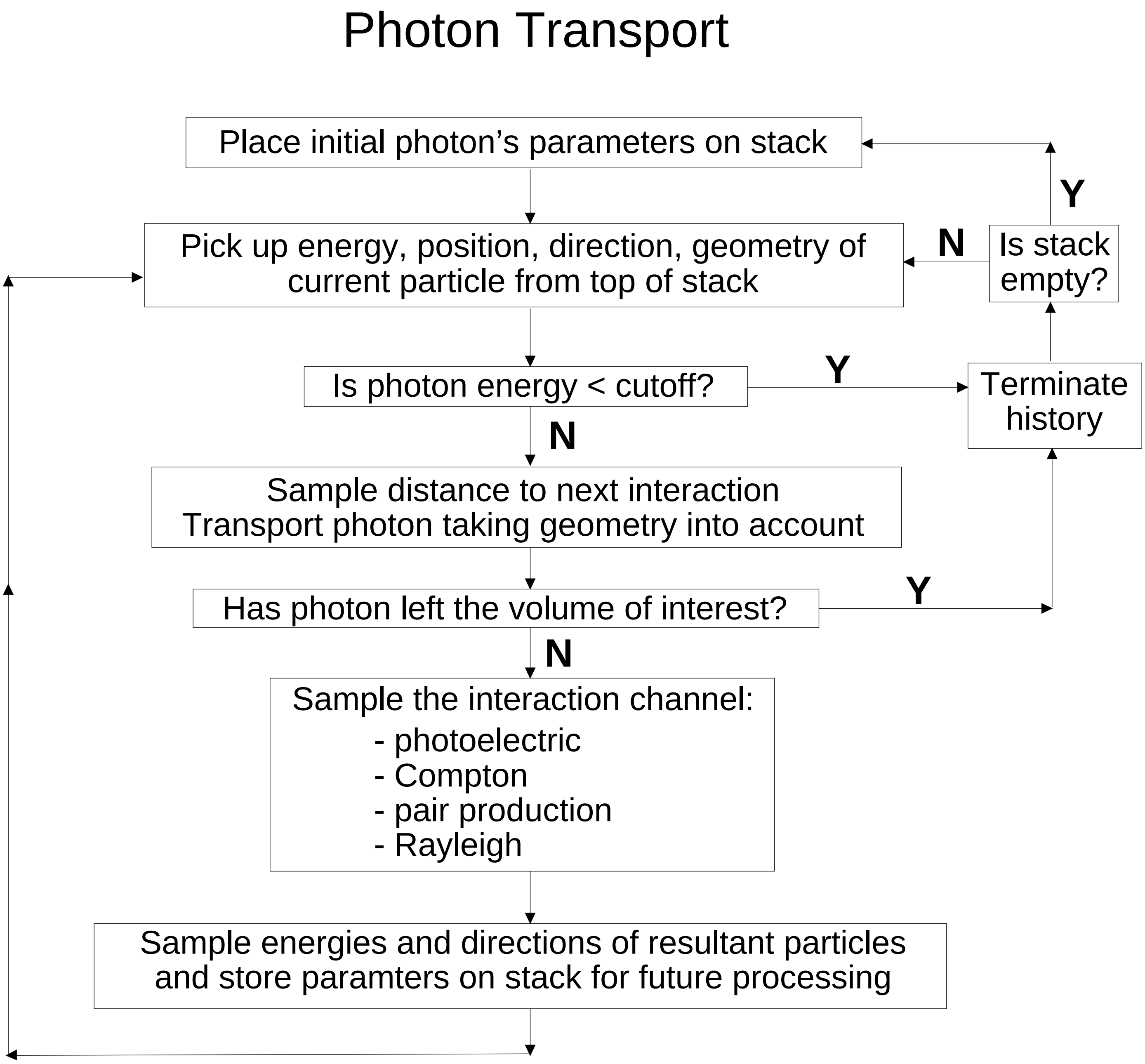

Figure 9: "Bare-bones" photon transport logic in EGS4.