Atmospheric Cascade Model

Oisín Morrison, under the supervision of Dr. Mark Lang (NUIG)

July 2020 - September 2020

This project was proposed as a summer internship project for NUIG's summer internship program in Physics. Following the cancellation of those internships owing to the Covid-19 pandemic, I took it on as a part-time research project.

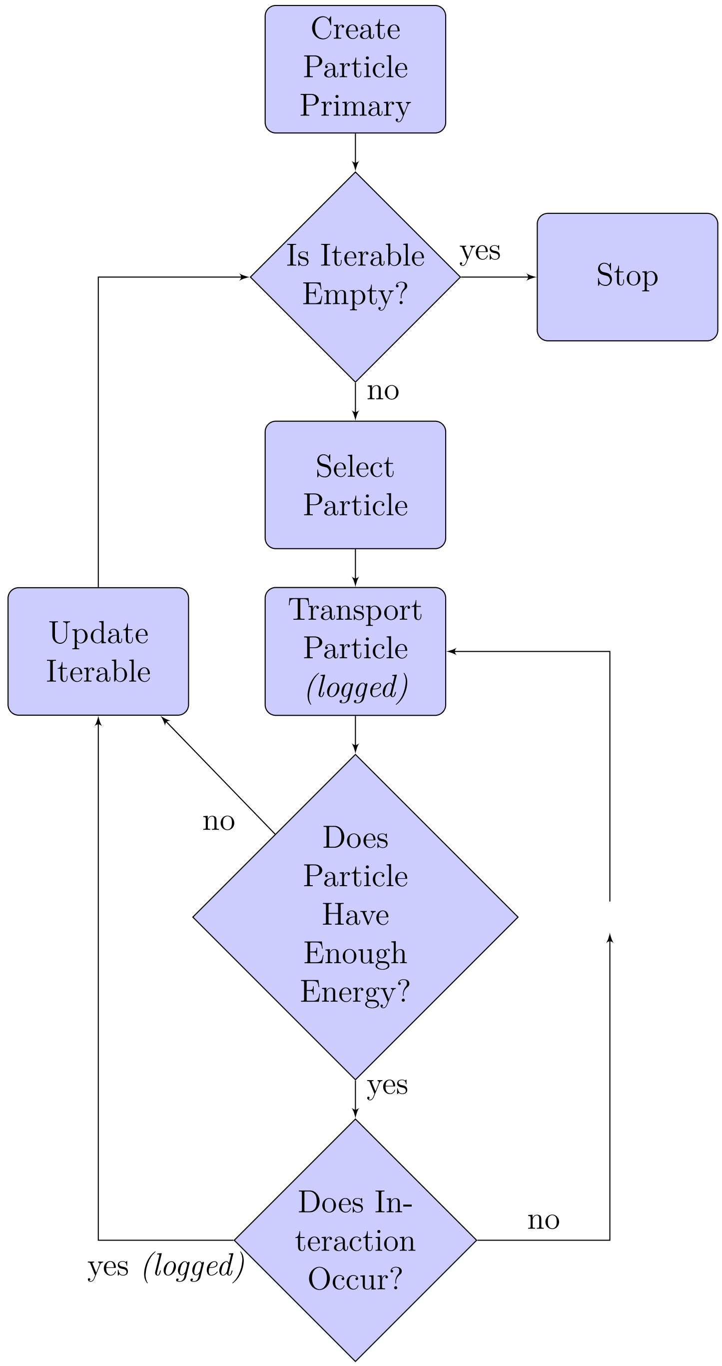
Contents

1 Introduction and Motivation

There do exist good tools to model atmospheric cascades, with Corsika being the most comprehensive. However, there do not exist good tools in Python for modelling this type of phenomenon. As a result, this project aimed to provide a way to model some atmospheric cascades solely in Python. We focused particularly on Cherenkov photons.

2 Overview of Model

This model has to take account of both the movement of the air shower and the various particle changes and interactions that occur. We can simulate the entire shower by simulating particle transport and particle interactions for a single particle at a time. The idea is that we have an iterable of particles (ordered by ascending energy), and then we take the first particle from the iterable and transport it until it interacts, reaches a boundary or has a low enough energy to be negligible. We then remove the particle from the iterable, add any newly produced particles to the iterable and repeat the process for the next particle in the iterable. When the iterable is empty, the simulation is complete. As a result, the general code flow is quite simple and can be summarised by the diagram on the next page.



Create Particle Primary
Is Iterable Empty?
yes
Stop
no
Select Particle
Update Iterable
Transport Particle *(logged)*
no
Does Particle Have Enough Energy?
yes
Does Interaction Occur?
no
yes *(logged)*

3 Notation and Techniques

3.1 Notation

I have chosen to mimic the notation used in the EGS4 documentation. All variables ζ_i thus refer to random numbers between 0 and 1 with a uniform probability distribution function.

3.2 Techniques

This model uses Monte-Carlo methods to simulate the behaviour of an air shower, and to do so it is necessary to sample probability density functions. A method which will show up repeatedly for sampling is the mixed method, which works as follows:

1. We put our function $\mathrm{f}(x)$ into the form $\sum_{i=1}^{n} \alpha_i \, \mathrm{f_i}(x) \, \mathrm{g_i}(x)$

2. We pick a random number between 0 and 1 and call it ζ_1. We select an i to be such that

$$\sum_{j=1}^{i-1} \alpha_j < \zeta_1 \sum_{j=1}^{n} \alpha_j \leq \sum_{j=1}^{n} \alpha_j$$

3. We select x by sampling $f_i(x)$, possibly via solving

$$\int_{-\infty}^{x} \mathrm{f_i}(x) \mathrm{d}x = \zeta_2$$

4. We randomly select ζ_3 and check if the condition $\zeta_3 < \mathrm{g_i}(x)$ is satisfied. If it is, we accept the value of x. If not, we go back to step 2.

The methods of sampling the f_i can also be via the mixed method.

4 Particle Transport

There are a few formulae we need to model particle transport. The mean free path λ is given by

$$\lambda = \frac{1}{\Sigma_t} = \frac{M}{N_\alpha \rho \sigma_t}$$

Thus, the probability of an interaction in a length dx is

$$\Pr(dx) = \frac{\mathrm{d}x}{\lambda}$$

Since in general the mean free path changes with different media or with energy loss, the number of mean free paths travelled will be given by an integral

$$N_\lambda = \int_{x_0}^{x} \frac{1}{\lambda(x)} \mathrm{d}x$$

It is then known that we can sample N_λ by using

$$N_\lambda = -\ln \zeta$$

The transport model is more complicated for charged particles. However, for photons, it is easy to understand.

4.1 Photons

First, we obtain the number of mean free paths travelled until the next interaction via $N_\lambda = -\ln \zeta$. Then we use this algorithm:

1. Compute λ at the given position.
2. Find $t_1 = \lambda N_\lambda$.
3. Find d, the distance to the closest boundary along the photon's current direction.
4. Find $t_2 = \min(t_1, d)$. Move the photon by a distance of t_2.
5. Find $z = N_\lambda - \frac{t_2}{\lambda}$.
6. If $z = 0$ (i.e. $t_2 = t_l$), then an interaction occurs and must be dealt with.
7. If $z > 0$ i.e. $t_2 = d$, then a boundary was reached and the process needs to be repeated. If the new region is a different material, Step 1 must be recomputed. Otherwise we can skip to Step 2.

4.2 Charged Particles

Photon transport was easy to simulate since the photons do not have that many possible interactions and thus we can simply partition what happens into: 1. travel in a straight line or 2. undergo an interaction. If we tried this approach for charged particles, we would have far too many interactions to deal with since some of the interactions' cross sections become very large as the transferred energy tends to zero. This is computationally infeasible for obvious reasons. Since the low energy transfer interactions which have these high cross-sections do not greatly affect the cascade's behaviour, we distinguish between these and interactions with higher energy transfers. We deal with high energy transfers in a discrete manner as before, but low energy transfers are dealt in a continuous manner and grouped together. The effect of this is that continuous energy loss means the cross section varies along the particle's path and the particle's path is furthermore no longer straight. There is a way to deal with this.
Note: To avoid confusion when I use the term "interaction", I shall henceforth call low energy interactions "scatterings" and I shall reserve the word "interactions" solely for high energy interactions.

The idea is namely to introduce a new cross section for a fictitious interaction which we call "straight ahead scattering" i.e. no interaction. This cross section is defined to be such that the total cross section is constant along the path i.e.

$$\sigma_{t,fic}(x) = \sigma_{t,real}(x) + \sigma_{fic}(x) = \text{constant} = \sigma_{t,real}(x_0)$$

As before we firstly obtain the number of mean free paths travelled until the next interaction via $N_\lambda = -\ln\zeta$. We then find the distance travelled using $N_\lambda = \int_{x_0}^{x} \frac{1}{\lambda(x)}\mathrm{d}x$, also using $\sigma_{t,fic}$. We can use this information to determine if an interaction occurs after the sampled distance, but first we have to take account of the continuous interactions that occur along the path's journey since these will change the particle's energy, thus affecting the cross sections.

4.2.1 Simulation of Scatterings

The path is subdivided into multiple small straight-line sections. The direction of travel of the particle is updated at the end of each of these small paths, as is the energy. Determining to what degree the direction should be changed is difficult. Determining the energy loss is simpler and I shall detail this first.

We are interested in how the energy changes with distance travelled. Thus, the formula of interest is:

$$-\left(\frac{\mathrm{d}E_{\pm}}{\mathrm{d}x}\right)_{\text{Continuous}} = -\left(\frac{\mathrm{d}E_{\pm}}{\mathrm{d}x}\right)_{\text{Soft Brems}} - \left(\frac{\mathrm{d}E_{\pm}}{\mathrm{d}x}\right)_{\text{Sub-Cutoff Electrons}}$$

The soft Bremsstrahlung term is constant for both electrons and positrons, and is given by integrating up to the cutoff energy A_p:

$$-\left(\frac{\mathrm{d}\check{E}}{\mathrm{d}x}\right)_{\text{Soft Bremsstrahlung}} = \int_0^{A_p} \check{k}\left(\frac{\mathrm{d}\check{\Sigma}_{Brem}}{\mathrm{d}\check{k}}\right)\mathrm{d}\check{k}$$

Note: A discussion of finding the cross-section for Bremsstrahlung can be found in the section about Bremsstrahlung within Particle Interactions (Section 5.1), so I shall not repeat myself here.

Similarly, for atomic electrons, we have:

$$-\left(\frac{\mathrm{d}E_{\pm}}{\mathrm{d}x}\right)_{\text{Sub-Cutoff Atomic Electrons}} = \int_0^{T_{max}} T\left(\frac{\mathrm{d}\Sigma_{\pm}}{\mathrm{d}T}\right)\mathrm{d}T$$

We can use some approximations to obtain a more useful formula:

$$\left(-X_0\frac{\mathrm{d}\check{E}_{\pm}}{\mathrm{d}x}\right)_{\text{Sub-Cutoff Atomic Electrons}} = \frac{X_0 n 2\pi r_0^2 m}{\beta^2}\left(\ln\frac{2(r+2)}{(I_{adj}/m)} + F^{\pm}(r,\Delta) - \delta\right)$$

where

$$F^{-}(r,\Delta) = -1-\beta^2+\ln\left((r-\Delta)\Delta\right)+\frac{r}{r-\Delta}+\gamma^{-2}\left[\frac{\Delta^2}{2}+(2r+1)\ln\left(1-\frac{\Delta}{r}\right)\right]$$

$$F^{+}(r,\Delta) = \ln(r\Delta)-\frac{\beta^2}{r}\left[r+2\Delta-1.5\Delta^2 y-\left(\Delta-\frac{\Delta^3}{3}\right)y^2-\left(\frac{\Delta^2}{2}-\frac{r\Delta^3}{3}+\frac{\Delta^4}{4}\right)y^3\right]$$

$$\gamma = \frac{\check{E}_0}{m}$$

$$r = \gamma - 1$$

$$\beta = \sqrt{1-\gamma^{-2}} = \frac{v}{c}$$

$$y = (\gamma+1)^{-1}$$

$$\Delta = \min(T'_E, T'_{max})$$

$$T'_E = \frac{T_E}{m_e} = \text{Kinetic energy cutoff in electron mass units}$$

$$T'_{max} = \begin{cases} r & \text{if positron} \\ \frac{r}{2} & \text{if electron} \end{cases}$$

$$\ln I_{adj} = \frac{\left(\sum_{i=1}^{N_e} p_i Z_i \ln\left(I_{adj}(Z_i)\right)\right)}{\left(\sum_{i=1}^{N_e} p_i Z_i\right)}$$

$$\delta = \begin{cases} 0 & x < x_0 \\ 2(\ln 10)x + C + a(x_1 - x)^{m_s} & x \in [x_0, x_1] \\ 2(\ln 10)x + C & x > x_1 \end{cases}$$

$$x = \log_{10}\left(\frac{\check{p}c}{m}\right) = \frac{\ln\eta}{\ln 10}$$

$$\eta = \sqrt{\gamma^2 - 1} = \beta\gamma = \frac{\check{p}_0 c}{m}$$

$$C = -2\ln\left(\frac{I_{adj}}{hv_P}\right) - 1$$

$$v_P = \sqrt{\frac{n r_0^2 c^2}{\pi}}$$

The other necessary constants e.g. m_s are obtained via tabulated values.

The direction of a particle is determined by Θ and ϕ. To simulate scattering, we just need to have these angles change. For Θ, we can sample from a probability density function dependent upon the material, particle energy and distance travelled. ϕ is simply chosen randomly. The direction of the particle is then adjusted.

The probability density function for Θ is

$$\mathrm{f}(\Theta) = \mathrm{f_M}(\Theta)\left(\mathrm{sinc}(\Theta)\right)^{1/2}$$

By defining

$$\theta = \frac{\Theta}{X_c B^{1/2}}$$

we can obtain

$$\mathrm{f_M}(\Theta)\mathrm{d}\Theta = \mathrm{f_r}(\theta)\mathrm{d}\theta$$

Now it is possible to sample the probability density function $\mathrm{f_M}(\Theta)$ by first sampling θ from its probability density function $\mathrm{f_r}(\theta)$ and then calculating Θ from θ. We reject all sampled $\Theta > \pi$. So, we just need $\mathrm{f_r}(\theta)$, which we can obtain from the first three terms of Bethe's Equation as:

$$\mathrm{f_r}(\theta) = \left[\mathrm{f}^0(\theta) + \frac{1}{B}\,\mathrm{f}^1(\theta) + \frac{1}{B^2}\,\mathrm{f}^2\right]\theta$$

where

$$\mathrm{f^n}(\theta) = \frac{1}{n!}\int_0^\infty u\mathrm{d}u\,\mathrm{J}_0(u\theta)e^{-0.25u^2}\left(0.25u^2\ln(0.25u^2)\right)^n$$

This function is horrible, so we use the mixed method to sample it rather than sampling directly. We use a factorisation for $\mathrm{f_r}(\theta)$ as follows:

$$\mathrm{f_r}(\theta) = \sum_{i=1}^{3} \alpha_i\,\mathrm{f_i}(\theta)\,\mathrm{g_i}(\theta)$$

where

$$\alpha_1 = 1 - \frac{\lambda}{B}$$

$$\mathrm{f}_1(\theta) = 2e^{-\theta^2}\theta$$

$$\mathrm{g}_1(\theta) = 1$$

$$\alpha_2 = 1 - \frac{\mu g_{2,Norm}}{B}$$

$$\mathrm{f}_2(\theta) = \frac{1}{\mu}$$

$$\mathrm{g}_2(\theta) = \frac{\theta}{g_{2,Norm}}\left(\lambda\,\mathrm{f}^0(\theta) + \mathrm{f}^1(\theta) + \frac{\mathrm{f}^2(\theta)}{B}\right)$$

$$\alpha_3 = 1 - \frac{g_{3,Norm}}{2\mu^2 B}$$

$$\mathrm{f}_3(\theta) = 2\mu^2\theta^{-3}$$

$$\mathrm{g}_3(\theta) = \frac{\theta^4}{g_{3,Norm}}\left(\lambda\,\mathrm{f}^0(\theta) + \mathrm{f}^1(\theta) + \frac{\mathrm{f}^2(\theta)}{B}\right)$$

The values for the constants were chosen to be:

$$\lambda = 2,\ \mu = 1,\ g_{2,Norm} = 1.80,\ g_{3,Norm} = 4.05$$

We also need to determine values for B and X_c. To do this, we can use the formulae below:

$$B = \begin{cases} \frac{2}{2-\ln 2}b & b < 2-\ln 2 \\ B > 1 \text{ satisfying } B - \ln(B) = b & b \geq 2 - \ln 2 \end{cases}$$

$$b = \ln(\Omega_0)$$

$$\Omega_0 = \frac{b_c t}{\beta^2}$$

$$b_c = \frac{\text{'6800'}\rho Z_S e^{\frac{Z_E}{Z_S}}}{M e^{\frac{Z_X}{Z_S}}}$$

$$\text{'6800'} = 4\pi N_a \left(\frac{h}{2\pi m_e c}\right)^2 \left[\frac{0.885^2}{1.167 \times 1.13}\right] = 6702.33$$

$$X_c = \frac{X_{cc}\sqrt{t}}{\check{E}_{MS}\beta^2}$$

$$X_{cc} = \frac{\text{'22.9'}\ \pi}{180}\sqrt{\frac{\rho Z_S}{M}}$$

$$\text{'22.9'} = \frac{180}{\pi}\sqrt{4\pi N_a} r_0 m = 22.696$$

$$Z_S = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_{MS}\right)$$

$$Z_E = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_{MS}\right) \ln Z_i^{-2/3}$$

$$Z_X = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_{MS}\right) \ln\left(1 + 3.34\left(\alpha Z_i\right)^2\right)$$

$$\beta = \sqrt{1-\gamma^{-2}} = \frac{v}{c}$$

The $\check{E}_{MS}$ term in the expression for X_c is the energy of the particle at the current step, and thus is not constant along the entire path. I have already discussed how to simulate the loss of energy along the path.

The idea is now we can sample these functions as according to the mixed method technique, but there are more caveats relating to how we do this. To sample $\mathrm{f}_1(\theta)$, we use:

$$\theta = \sqrt{-\ln\zeta}$$

$\mathrm{f}_2(\theta)$ is sampled by merely choosing a uniformly distributed random number i.e.

$$\theta = \zeta$$

Lastly, to sample $\mathrm{f}_3(\theta)$, we have a more complicated procedure. To get θ in that case, we firstly sample $\eta = \frac{1}{\theta}$ using:

$$\mathrm{f}_{\eta 3}(\eta) = 2\mu^2\eta$$

and

$$\mathrm{g}_{\eta 3}(\eta) = \frac{\eta^{-4}}{g_{3,Norm}}\left(\lambda\,\mathrm{f}^0\left(\frac{1}{\eta}\right) + \mathrm{f}^1\left(\frac{1}{\eta}\right) + \frac{\mathrm{f}^2\left(\frac{1}{\eta}\right)}{B}\right)$$

To sample $\mathrm{f}_{\eta 3}(\eta)$, we take the larger of two random numbers i.e.

$$\eta = \max(\zeta_1, \zeta_2)$$

Then we convert our sampled η back to θ.

4.2.2 Interaction Determination

Once we have travelled the sampled distance, we need to determine whether an interaction occurs. To do this, a random number is chosen. If it is larger than

$$\frac{\sigma_{t,real}(x)}{\sigma_{t,real}(x_0)} = \frac{\Sigma_{t,real}(x)}{\Sigma_{t,real}(x_0)}$$

then the interaction is deemed fictitious and the transport is continued without interaction. Otherwise, the interaction is real and has to be dealt with.

4.2.3 Travel Length

This method of dealing with scatterings is only approximate and as a result the distances over which we conduct the approximation must be limited i.e. we need to split up our dx into multiple smaller sections.
The condition we use on our path length is that the distance t travelled in a step satisfies

$$t < t_{P_{max}} = t_s(\check{E})\varepsilon_{P_{max}}$$

where

$$\varepsilon_{P_{max}} = 0.3$$

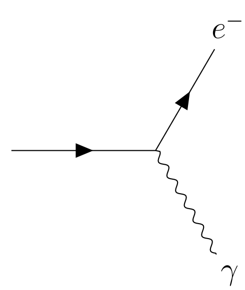
$$t_s(\check{E}) = X_0 \left(\frac{2\check{E}\beta^2}{\check{E}_s}\right)$$

$$\check{E}_s = m\sqrt{\frac{4\pi}{\alpha}} = 21.2$$

5 Particle Interaction

5.1 Bremsstrahlung

The Feynman diagram for this process is shown below:



We call the energy of the incident particle E_0, the energy of the emitted photon k and the energy of the emitted particle is denoted E. The formula for the differential cross section is then given by:

$$\frac{\mathrm{d}\sigma_{Brem}(Z,\check{E}_0,\check{k})}{\mathrm{d}\check{k}} = \frac{A'(Z,\check{E}_0)r_0^2\alpha Z(Z+\xi(Z))}{\check{k}}\times$$
$$\left(\left[1+\left(\frac{\check{E}}{\check{E}_0}\right)^2\right]\left[\phi_1(\delta)-\frac{4}{3}\ln Z-\big(4\,\mathrm{f_c}(Z)\text{ if }\check{E}_0>50,0\big)\right]-\right.$$
$$\left.\frac{2\check{E}}{3\check{E}_0}\left[\phi_2(\delta)-\frac{4}{3}\ln Z-\big(4\,\mathrm{f_c}(Z)\text{ if }\check{E}_0>50,0\big)\right]\right)$$

where

$$E_0 = k + E$$

$$\delta = 272Z^{-1/3}\Delta$$

$$\Delta = \frac{\check{k}m}{2\check{E}_0\check{E}}$$

$$\phi_1 = \begin{cases} 20.867 - 3.242\delta + 0.625\delta^2 & \delta \leq 1 \\ 21.12 - 4.184\ln(\delta + 0.952) & \delta > 1 \end{cases}$$

$$\phi_2 = \begin{cases} 20.029 - 1.930\delta + 0.086\delta^2 & \delta \leq 1 \\ 21.12 - 4.184\ln(\delta + 0.952) & \delta > 1 \end{cases}$$

$$\mathrm{f_c}(Z) = a^2\left[\left(1+a^2\right)^{-1} + 0.20206 - 0.0369a^2 + 0.0083a^4 - 0.002a^6\right]$$

$$a = \alpha Z$$

$$\xi(Z) = \frac{L'_{rad}(Z)}{L_{rad}(Z) - \mathrm{f_c}(Z)}$$

$$L'_{rad}(Z) = \begin{cases} 6.144 & Z = 1 \\ 5.621 & Z = 2 \\ 5.805 & Z = 3 \\ 5.924 & Z = 4 \\ \ln(1194Z^{-2/3}) & Z > 4 \end{cases}$$

$$L_{rad}(Z) = \begin{cases} 5.310 & Z = 1 \\ 4.790 & Z = 2 \\ 4.740 & Z = 3 \\ 4.710 & Z = 4 \\ \ln(184.15Z^{-1/3}) & Z > 4 \end{cases}$$

For $\check{E}_0 > 50$, $A'(Z, \check{E}_0) = 1$. To find values when $\check{E}_0 \leq 50$, we should use tabulated values (possibly from https://physics.nist.gov/PhysRefData/Xcom/Text/intro.html). However, I have just assumed that it is always 1 for now.
Changing notation to x_0 and x such that $x_0 = \check{E}_0$ and $x = \check{k}$, we clearly have a corrected and uncorrected differential cross-section related by:

$$\frac{\mathrm{d}\sigma_{corrected}(Z, x_0, x)}{\mathrm{d}x} = A'(Z, x_0)\frac{\mathrm{d}\sigma_{uncorrected}(Z, x_0, x)}{\mathrm{d}x}$$

Thus, the macroscopic differential cross section will be given by:

$$\frac{\mathrm{d}\Sigma(x_0, x)}{\mathrm{d}x} = \frac{N_a\rho}{M}\sum_{i=1}^{N_e} p_i \frac{\mathrm{d}\sigma_{corrected}(Z_i, x_0, x)}{\mathrm{d}x}$$

And the total macroscopic cross section is:

$$\Sigma(x_0) = \int_{x_{min}}^{x_{max}} \frac{\mathrm{d}\Sigma(x_0, x)}{\mathrm{d}x}\mathrm{d}x$$

where $x_{min} = A_P$ and $x_{max} = \check{E}_0 - m$.

The probability density function for secondary particle energy is then as follows:

$$\mathrm{f}(x) = \frac{\mathrm{d}\Sigma(x_0, x)}{\mathrm{d}x}\bigg/\Sigma(x_0)$$

We use the mixed method to sample this function. To do this, we sample

$$\varepsilon = \frac{\check{k}}{\check{E}_0} = \frac{x}{x_0}$$

and then convert back. Note that any constants in front of the probability density function don't matter, so with this in mind we can use the following equation:

$$\frac{\mathrm{d}\check{\Sigma}}{\mathrm{d}\varepsilon} = \frac{Z_A + Z_B - \left(Z_F \text{ if } \check{E}_0 > 50, 0\right)}{Z_{AB} - Z_F}\times$$
$$\left(\left[\ln 2\left(\frac{4}{3} + \frac{1}{9\ln 184.15\left[1 + \left(Z_U \text{ if } \check{E}_0 > 50, Z_P\right)\right]}\right)\right]\times\right.$$
$$\left.\frac{1}{\ln 2}\frac{1-\varepsilon}{\varepsilon}A(\delta') + \varepsilon B(\delta')\right)$$

where

$$\frac{\mathrm{d}\check{\Sigma}}{\mathrm{d}\varepsilon} = X_0 \frac{\mathrm{d}\Sigma}{\mathrm{d}\varepsilon}$$

$$X_0(Z)^{-1} = \frac{N_a \rho \alpha r_0^2}{A} \left[Z^2 \left(L_{rad}(Z) - f_c(Z) \right) + Z L'_{rad}(Z) \right]$$

$$Z_A = Z_T \ln 184.15$$

$$Z_T = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_i \right)$$

$$Z_B = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_i \right) \ln \left(Z_i^{-1/3} \right)$$

$$Z_F = \sum_{i=1}^{N_e} p_i Z_i \left(Z_i + \xi_i \right) f_c(Z_i)$$

$$Z_U = \frac{Z_B - Z_F}{Z_A}$$

$$\delta' = \Delta_E \Delta_C$$

$$\Delta_E = \frac{1 - \varepsilon}{\varepsilon \check{E}_0}$$

$$\Delta_C = 136 m e^{Z_G}$$

$$A(\delta') = \frac{3\phi_1(\delta') - \phi_2(\delta') + 8 \left(Z_V \text{ if } \check{E}_0 > 50, Z_G \right)}{\frac{2}{3} + 8 \left[\ln 184.15 + \left(Z_V \text{ if } \check{E}_0 > 50, Z_G \right) \right]}$$

$$B(\delta') = \frac{\phi_1(\delta') + 4 \left(Z_V \text{ if } \check{E}_0 > 50, Z_G \right)}{4 \left[\ln 184.15 + \left(Z_V \text{ if } \check{E}_0 > 50, Z_G \right) \right]}$$

$$Z_V = \frac{Z_B - Z_F}{Z_T}$$

$$Z_G = \frac{Z_B}{Z_T}$$

$$Z_P = \frac{Z_B}{Z_A}$$

$$\phi_1 = \begin{cases} 20.867 - 3.242\delta + 0.625\delta^2 & \delta \leq 1 \\ 21.12 - 4.184 \ln \left(\delta + 0.952 \right) & \delta > 1 \end{cases}$$

$$\phi_2 = \begin{cases} 20.029 - 1.930\delta + 0.086\delta^2 & \delta \leq 1 \\ 21.12 - 4.184\ln(\delta + 0.952) & \delta > 1 \end{cases}$$

Z_{AB} is not given and not required since the decomposition we will use does not include it. To find X_0 for composite materials, we can use the following formula from https://www-physics.lbl.gov/ gilg/PixelUpgradeMechanicsCooling/Material/Radiationlength.pdf:

$$X_0^{-1} = \sum_{i=1}^{N_e} A_i X_0(Z_i, A_i)^{-1}$$

Again, since the constants don't matter, we can decompose the function for the purposes of sampling the secondary energy via the mixed method. The functions we use to do this are:

$$\alpha_1 = \ln 2 \left(\frac{4}{3} + \frac{1}{9 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{E}_0 > 50, Z_P \right) \right]} \right)$$

$$\mathrm{f}_1(\varepsilon) = \frac{1}{\ln 2} \frac{1 - \varepsilon}{\varepsilon}$$

$$\mathrm{g}_1(\varepsilon) = \left(A(\delta'(\varepsilon)) \text{ if } \varepsilon \check{E}_0 \in (A_P, \check{E}_0 - m), 0 \right)$$

$$\alpha_2 = \frac{1}{2}$$

$$\mathrm{f}_2(\varepsilon) = 2\varepsilon$$

$$\mathrm{g}_2(\varepsilon) = \left(B(\delta'(\varepsilon)) \text{ if } \varepsilon \check{E}_0 \in (A_P, \check{E}_0 - m), 0 \right)$$

As always, we now need to figure out a way to sample f_1 and f_2. For f_2, this is simple and we simply take the largest of two random numbers i.e.

$$\varepsilon = \max(\zeta_1, \zeta_2)$$

For f_1, we have an issue since it has an infinite integral over $(0, 1)$. To get around this, we limit the interval upon which f_1 is sampled to $(2^{-N_{Brem}}, 1)$, where N_{Brem} satisfies:

$$2^{-N_{Brem}} \leq \frac{A_P}{\check{E}_0} < 2^{-N_{Brem}+1}$$

To sample f_1, we further factorise it to:

$$f_1(\varepsilon) = \sum_{j=0}^{N_{Brem}} \alpha_{1j} f_{1j}(\varepsilon) g_{1j}(\varepsilon)$$

where

$$\alpha_{1j} = 1$$

$$f_{1j}(\varepsilon) = \begin{cases} \frac{1}{\ln 2} 2^{j-1} & \varepsilon \leq 2^{-j} \\ \frac{1}{\ln 2} \frac{1-\varepsilon 2^{j-1}}{\varepsilon} & 2^{-j} < \varepsilon < 2^{-j+1} \\ 0 & \varepsilon \geq 2^{-j+1} \end{cases}$$

$$g_{1j}(\varepsilon) = 1$$

Then, to sample f_1 we first select a subdistribution index j using

$$j = \text{Integer Part}(N_{Brem}\zeta_1) + 1$$

The next step is to sample f_{1j}. To do this, we define:

$$p = 2^{1-j}$$

and

$$\varepsilon' = \frac{\varepsilon}{p}$$

We then convert our probability density function to be one of ε', defined as:

$$g(\varepsilon') = \begin{cases} \frac{1}{\ln 2} & \varepsilon' \in \left(0, \frac{1}{2}\right) \\ \frac{1}{\ln 2} \frac{1-\varepsilon'}{\varepsilon'} & \varepsilon' \in \left(\frac{1}{2}, 1\right) \end{cases}$$

Once more, we factorise this as:

$$g(\varepsilon') = \sum_{i=1}^{2} \alpha'_i f'_i(\varepsilon') g'_i(\varepsilon')$$

where

$$\alpha'_1 = \frac{1}{2 \ln 2}$$

$$f'_1(\varepsilon') = \begin{cases} 2 & \varepsilon' \in \left(0, \frac{1}{2}\right) \\ 0 & \varepsilon' \in \left(\frac{1}{2}, 1\right) \end{cases}$$

$$g'_1(\varepsilon') = 1$$

$$\alpha'_2 = 1 - \frac{1}{2\ln 2}$$

$$f'_2(\varepsilon') = \begin{cases} 0 & \varepsilon' \in \left(0, \frac{1}{2}\right) \\ \frac{1}{\ln 2 - 0.5}\frac{1-\varepsilon'}{\varepsilon'} & \varepsilon' \in \left(\frac{1}{2}, 1\right) \end{cases}$$

$$g'_2(\varepsilon') = 1$$

Finally, we can sample these. For $f'_1(\varepsilon')$, we draw a random number and half it i.e.

$$\varepsilon' = \frac{\zeta}{2}$$

To sample $f'_2(\varepsilon')$, we let $\varepsilon' = 1 - 0.5x$ and we sample x from:

$$h(x) = \alpha'' f''(x) g''(x)$$

where

$$\alpha'' = \frac{1}{4\ln 2 - 2}$$

$$f''(x) = 2x$$

$$g''(x) = \frac{1}{2-x} = 12\varepsilon'$$

We already know that to sample a function like $f''(x)$ since this was our $f_2(\varepsilon)$. Namely, we get the maximum of two random numbers i.e.

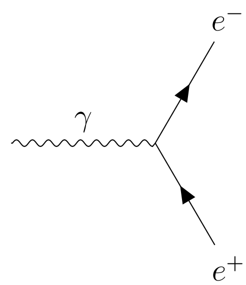
$$x = \max(\zeta_1, \zeta_2)$$

Thus, we finally have a way of sampling the secondary energies after this interaction.

One also has to worry about the direction of emission of the particles. We assume the electron direction of travel is unchanged, and we take θ of the emitted photon to be $\theta = \frac{m}{E_0}$ relative to the incident electron. The azimuthal angle ϕ is chosen randomly.

5.2 Pair Production

The Feynman diagram for this process is shown below:



We call the energy of the γ ray k and the energies of the electron and positron E_- and E_+ respectively. The formula for the differential cross section is then given by:

$$\frac{\mathrm{d}\sigma_{Pair}(Z,\check{k},\check{E}_+)}{\mathrm{d}\check{E}_+} = \frac{A'_p(Z,\check{k}) r_0^2 \alpha Z(Z+\xi(Z))}{\check{k}^3} \times$$
$$\left(\left[\check{E}_+^2 + \check{E}_-^2\right] \left[\phi_1(\delta) - \frac{4}{3}\ln Z - \left(4\,\mathrm{f_c}(Z) \text{ if } \check{k} > 50, 0\right)\right] + \right.$$
$$\left. \frac{2}{3}\check{E}_+\check{E}_- \left[\phi_2(\delta) - \frac{4}{3}\ln Z - \left(4\,\mathrm{f_c}(Z) \text{ if } \check{k} > 50, 0\right)\right]\right)$$

where

$$k = E_+ + E_-$$
$$\delta = 272 Z^{-1/3}\Delta$$
$$\Delta = \frac{\check{k}m}{2\check{E}_+\check{E}_-}$$
$$\phi_1 = \begin{cases} 20.867 - 3.242\delta + 0.625\delta^2 & \delta \leq 1 \\ 21.12 - 4.184\ln(\delta + 0.952) & \delta > 1 \end{cases}$$
$$\phi_2 = \begin{cases} 20.029 - 1.930\delta + 0.086\delta^2 & \delta \leq 1 \\ 21.12 - 4.184\ln(\delta + 0.952) & \delta > 1 \end{cases}$$
$$\mathrm{f_c}(Z) = a^2\left[\left(1+a^2\right)^{-1} + 0.20206 - 0.0369a^2 + 0.0083a^4 - 0.002a^6\right]$$
$$a = \alpha Z$$
$$\xi(Z) = \frac{L'_{rad}(Z)}{L_{rad}(Z) - \mathrm{f_c}(Z)}$$

$$L'_{rad}(Z) = \begin{cases} 6.144 & Z = 1 \\ 5.621 & Z = 2 \\ 5.805 & Z = 3 \\ 5.924 & Z = 4 \\ \ln(1194Z^{-2/3}) & Z > 4 \end{cases}$$

$$L_{rad}(Z) = \begin{cases} 5.310 & Z = 1 \\ 4.790 & Z = 2 \\ 4.740 & Z = 3 \\ 4.710 & Z = 4 \\ \ln(184.15Z^{-1/3}) & Z > 4 \end{cases}$$

For $\check{E}_0 > 50$, $A'_p(Z, \check{E}_0) = 1$. To find values when $\check{E}_0 \leq 50$, we should use tabulated values.

To get the total cross-section, we change notation to x_0 and x such that $x_0 = \check{k}$ and $x = \check{E}_+$. We clearly have a corrected and uncorrected differential cross-section related by:

$$\frac{\mathrm{d}\sigma_{corrected}(Z, x_0, x)}{\mathrm{d}x} = A'_p(Z, x_0)\frac{\mathrm{d}\sigma_{uncorrected}(Z, x_0, x)}{\mathrm{d}x}$$

Thus, the macroscopic differential cross section will be given by:

$$\frac{\mathrm{d}\Sigma(x_0, x)}{\mathrm{d}x} = \frac{N_a \rho}{M} \sum_{i=1}^{N_e} p_i \frac{\mathrm{d}\sigma_{corrected}(Z_i, x_0, x)}{\mathrm{d}x}$$

And the total macroscopic cross section is:

$$\Sigma(x_0) = \int_{x_{min}}^{x_{max}} \frac{\mathrm{d}\Sigma(x_0, x)}{\mathrm{d}x} \mathrm{d}x$$

where $x_{min} = A_E$ and $x_{max} = \check{k} - m$.

As per the discussion for Bremsstrahlung, the probability density function for the secondary particle energies then comes from normalising the macroscopic differential cross section. As a result, to sample this function we can simply sample the differential cross section. To achieve this, we first switch to a new variable ε given by

$$\varepsilon = \frac{\check{E}_-}{\check{k}}$$

Then we have the following formula:

$$\begin{aligned}\frac{\mathrm{d}\check{\Sigma}}{\mathrm{d}\varepsilon} = {} & \frac{Z_A + Z_B - \left(Z_F \text{ if } \check{k} > 50, 0\right)}{Z_{AB} - Z_F} \times \\ & \left(\left[\frac{2}{3} - \frac{1}{36 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]} \right] C(\delta') + \right. \\ & \left[\frac{1}{12} \left(\frac{4}{3} + \frac{1}{9 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]} \right) \right] \times \\ & \left. 12 \left(\varepsilon - \frac{1}{2} \right)^2 A(\delta') \right)\end{aligned}$$

where

$$\delta' = \Delta_E \Delta_C$$

$$\Delta_E = \frac{1}{\check{k}\varepsilon\,(1-\varepsilon)}$$

$$C(\delta') = \frac{3\phi_1(\delta') + \phi_2(\delta') + 16\left(Z_V \text{ if } \check{k} > 50, Z_G\right)}{-\frac{2}{3} + \left(16 \ln 184.15 + \left(Z_V \text{ if } \check{k} > 50, Z_G\right)\right)}$$

and the other variables are the same as in the Bremsstrahlung case. We can ignore the first factor when sampling to be left with

$$\begin{aligned}\frac{\mathrm{d}\check{\Sigma}_{run-time}}{\mathrm{d}\varepsilon} = {} & \left(\left[\frac{2}{3} - \frac{1}{36 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]} \right] C(\delta') + \right. \\ & \left[\frac{1}{12} \left(\frac{4}{3} + \frac{1}{9 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]} \right) \right] \times \\ & \left. 12 \left(\varepsilon - \frac{1}{2} \right)^2 A(\delta') \right)\end{aligned}$$

To sample this we once again use the mixed method with the following factorisation:

$$\alpha_1 = \left[\frac{2}{3} - \frac{1}{36 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]} \right]$$

$$f_1(\varepsilon) = 1$$

$$g_1(\varepsilon) = \big(C(\delta'(\varepsilon)) \text{ if } \check{k}\varepsilon \in (m, \check{k} - m), 0\big)$$

$$\alpha_2 = \frac{1}{12}\left[\frac{4}{3} + \frac{1}{9 \ln 184.15 \left[1 + \left(Z_U \text{ if } \check{k} > 50, Z_P\right)\right]}\right]$$

$$f_2(\varepsilon) = 12\left(\varepsilon - \frac{1}{2}\right)^2$$

$$g_2(\varepsilon) = \big(A(\delta'(\varepsilon)) \text{ if } \check{k}\varepsilon \in (m, \check{k} - m), 0\big)$$

We spot that the pair production formula is symmetric about $\varepsilon = \frac{1}{2}$. One of the particles will be given energy $\check{k}\varepsilon$ and the other $\check{k}(1 - \varepsilon)$. The choice of which one is a positron is made randomly. We can restrict the range of ε sampled to $\left(0, \frac{1}{2}\right)$ and double f_1 and f_2 as is done in EGS4, but I have chosen not to do that.
Instead, we now sample f_1 as normal and without any doubling using:

$$\varepsilon = \zeta$$

f_2 can be sampled by:

$$\varepsilon = 1 - \max\left(\zeta_1, \zeta_2, \zeta_3\right)$$

This gives us our method for sampling the secondary energies.

One also has to worry about the direction of emission of the particles. We take θ of the emitted particles to be $\theta = \frac{m}{\check{k}}$ relative to the incident photon. The azimuthal angle ϕ is chosen randomly for one of the particles and then the other receives the negative of that angle.

5.3 Cherenkov Radiation

Cherenkov Radiation was implemented in the particle transport phase of the model. For each charged particle step, it was examined whether the condition $n\beta > 1$ was met. If it was, then Cherenkov photons were emitted. The angle θ_c relative to the incident charged particle of the emitted photons was given by:

$$\theta_c = \arccos\left(\frac{1}{n\beta}\right)$$

where

$$n \approx 1 + 0.000283 \times \frac{\rho(h)}{\rho(0)}$$

The azimuthal angle is chosen randomly. The number of photons emitted at this angle per path length s that are detectable in a range of wavelengths between λ_0 and λ_1 can be found from:

$$\frac{\mathrm{d}N_c}{\mathrm{d}s} = 2\pi\alpha \int_{\lambda_0}^{\lambda_1} \frac{\sin^2\theta_c}{\lambda^2} \mathrm{d}\lambda$$

which can be converted to:

$$N \approx 2\pi s\alpha \sin^2\theta_c \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_1}\right)$$

For computational efficiency, Cherenkov photons are considered in bunches for each of these movements as opposed to individual particles. They are also treated as non-interacting bodies and do not undergo any of the transport or interaction phases. Whether or not they hit the detector is extrapolated from their positions and directions.

6 The Codebase

There are three main folders in my repository - called HEITLER, EGS4 and MAIN. HEITLER contains my code for reproducing the Heitler model as per Matthews. The EGS4 repository contains my code for implementing the base functionality in EGS4 - only considering bremsstrahlung and pair production reactions. Finally, MAIN contains an improved version of my code in EGS4 with the addition of Cherenkov radiation simulation.

7 Closing Remarks

This was a relatively short and part-time project, so I did not get to fulfill everything I would have liked to do. The main issue to be reckoned with currently is the code execution time. Integrations to find the total cross sections or similar are computationally expensive, and because the mixed method for sampling is recursive this function can also be computationally expensive. To get around these, I would like to read tabular data on cross-sections rather than integrating each time, and I would like to add an exit functionality from the sampling after a high number of recursions which just takes the default, average values instead of a sampled one. Unfortunately I

have yet to implement these.
Nonetheless, I was able to implement the main EGS4 features in Python, along with Cherenkov radiation.

8 References

[1] W.R. Nelson, H. Hirayama and D.W.O. Rogers. *SLAC-265*. Stanford Linear Accelerator Center, 1985.

[2] H. Hirayama, Y. Namito, A.F. Bielajew, S.J. Wilderman and W.R. Nelson. *SLAC-R-730*. Stanford Linear Accelerator Center, 2005.

[3] I. Kawrakow, E. Mainegra-Hing, D.W.O. Rogers, F. Tessier and B.R.B. Walters. *The EGSnrc code system: Monte Carlo simulation of electron and photon transport, NRCC report PIRS-701*. NRC Canada, 2001–2015.

[4] D. Heck, J. Knapp, J.N. Capdevielle, G. Schatz, T. Thouw. *CORSIKA: A Monte Carlo Code to Simulate Extensive Air Showers*. Forschungszentrum Karlsruhe GmbH, Karlsruhe, 1998.

[5] R. Engel, D. Heck, T. Huege et al. *Towards A Next Generation of CORSIKA: A Framework for the Simulation of Particle Cascades in Astroparticle Physics*. Computing and Software for Big Science 3:2, 2019.

[6] J. Matthews. *A Heitler model of extensive air showers*. Astroparticle Physics, 22 (5-6) , pp. 387-397, 2005.

[7] A.T. Leclère. *An Evaluation of Bremsstrahlung Cross-Sections for keV to GeV Electrons*. University of Florida, 2001.