Simulating Compton Scattering using Monte Carlo method: COSMOC library

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ABSTRACT

In the following article we present properties and functionality of the COSMOC library designed to exploit basic features of Compton scattering process and its computational modelling. Basic physics of Compton scattering is pointed out, accompanied by various procedures accessible by user. The COSMOC library uses Monte Carlo method to perform single photon scattering. Special care is given to emphasize use of proper random number generator for Monte Carlo method.

Keywords: Monte Carlo – Compton scattering – C++

1 INTRODUCTION

Scattering of photons on free charged particle is called Compton scattering. It was first observed in year 1923 by Arthur H. Compton when he was examining scattering of X-ray photons on stationary electrons. The Compton scattering was found to be useful in many areas of science and astrophysics is no exception. Its influence can be found in spectra produced by many astrophysical objects and phenomena. This is especially true in low densities of matter where Compton scattering is dominating in comparison with other types of scatterings. By scattering on non-relativistic electrons the photons can only loose energy on the other hand scattering by relativistic electrons can result in increased energy of the scattered photons. Even moderately energetic electrons can contribute to the resulting spectra by multiple scatterings of photons, this behaviour is called comptonization.

The Compton scattering is suspected to be responsible for power law shaped spectra emitted by many astrophysical objects. Scattering of synchrotron photons is considered in explaining non-thermal (power law) parts of the spectra of sources like blazars or radio quasars. The comptonization has considerable effect in X-ray emission in hard (low) and soft (high) spectral states of black-hole binaries.

Effects of the Compton scattering on observed spectra can by more easily simulated by Monte Carlo method. One of the first Monte Carlo simulations of the Compton scattering and its effect on observed spectra is work by (Pozdnyakov et al., 1983). Full relativistic treatment of the Compton scattering was recently done by (Dolence et al., 2009) or

(Schnittman and Krolik, 2013). Polarisation was also introduced into Compton scattering codes, for more details see works by (McNamara et al., 2008) or (Krawczynski, 2012). Aim of our code is to calculate Compton scattering in Kerr space-time with help of Monte Carlo method. The code is in form of C library.

This library is concerned only with Compton scattering on free electrons and does not consider any modifications needed for scatterings on bounded electrons. It is also limited to gases which can be approximated by equation of state for ideal gas. It also does not consider polarization. Polarization should be first candidate for improvements of the library in the future. The COSMOC library was written using GSL 1.16. The GSL is an abbreviation of GNU Scientific Library and it is a numerical library for C and C++. It provides wide variety of numerical methods for scientific purposes.

2   COMPTON SCATTERING

2.1   Compton Scattering

The Compton scattering is an inelastic scattering process, where photon is scattered by free charged particle, usually electron. Since the scattering is inelastic photon looses energy in favour of the scattering particle. The differential cross-section is described by the Klein–Nishina formula (Rybicki and Lightman, 1985)

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}r_0^2\frac{\epsilon_f^2}{\epsilon_i^2}\left(\frac{\epsilon_i}{\epsilon_f} + \frac{\epsilon_f}{\epsilon_i} - \sin^2(\theta)\right), \tag{1}$$

where r_0 is classical electron radius, ϵ_i is the energy of the incident photon and ϵ_f is the energy of the scattered photon. This equation also gives probability distribution function $\mathrm{pdf}_C(\theta)$ for scattering angle θ of the Compton scattering.

The energy of the scattered photon is given by following relationship (Rybicki and Lightman, 1985)

$$\epsilon_f = \frac{\epsilon_i}{1 + \frac{\epsilon_i}{m_e c^2}\left(1 - \cos(\theta)\right)}. \tag{2}$$

The total cross-section is an integral of differential cross-section (1) over spatial angle Ω and it is given by

$$\sigma = \int \frac{d\sigma}{d\Omega}d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \frac{d\sigma}{d\Omega}\sin(\theta). \tag{3}$$

After we perform integration we arrive at (Rybicki and Lightman, 1985)

$$\sigma = \sigma_{\mathrm{T}}\frac{3}{4}\left[\frac{1+x}{x^3}\left(\frac{2x(1+x)}{1+2x} - \ln(1+2x)\right) + \frac{1}{2x}\ln(1+2x) - \frac{1+3x}{(1+2x)^2}\right], \tag{4}$$

where $x = \epsilon_i/(m_e c^2)$ and $\sigma_{\mathrm{T}} = (8\pi/3)r_0^2$ is Thomson total cross-section.

To obtain cumulative distribution function $\text{cdf}_C(\theta)$ we must integrate Eq. (1) over scattering angle θ, where ϵ_f is given by Eq. (2). This gives

$$\text{cdf}_C(\theta) = \frac{r_0^2}{4x^2}\left[2\theta - \frac{2B\arctan\left(-\sqrt{1+2x}\tan(\theta/2)\right)}{\sqrt{(1+2x)^5}}\right] +$$

$$+ \frac{r_0^2}{4x^2}\left[\frac{x^3\sin(\theta)}{(1+2x)\left(1+x\left(1-\cos(\theta)\right)\right)^2}\right] + \frac{r_0^2}{4x^2}\left[\frac{x\left(3x^3 + 11x^2 + 8x + 2\right)\sin(\theta)}{(1+2x)^2\left(1+x\left(1-\cos(\theta)\right)\right)}\right],$$

$$(5)$$

where $B = 11x^4 + 4x^3 - 12x^2 - 10x - 2$.

Implementation in the code

The implementation of Compton scattering consists of following subroutines. Equation (1) can be invoked by calling function `CM_diffcr`, total cross-section Eq. (4) is returned by function `CM_totcr`. To obtain values of the $\text{cdf}_C(\theta)$ for different values of scattering angle θ one must call function `CM_EDiE_cdf`. These functions are used by procedure for generating random numbers with Klein–Nishina distribution `Random_num_icdf_bisection_CM_EDiE`. This function implements bisection to search for value of the inverse $\text{cdf}_C(\theta)$ and produces one random number per call.

2.2   Thomson Scattering

The Thomson scattering is a special case of Compton scattering, it is an approximation of the Compton scattering for low photon energies. This approximation can be used as long as incident photon energies $\epsilon_i \ll 511\,\text{keV}$ (electron rest energy). The differences in probability distribution functions $\text{pdf}_C(\theta)$ for distinct photon energies are shown in the Figure 1. Since energy of the incident photon is much smaller than electron rest energy $\epsilon_i \ll m_e c^2$ we can neglect denominator in Eq. (2) and get

$$\epsilon_f = \epsilon_i,\qquad(6)$$

which means that photon energy ϵ_i is not changed by the scattering. Using this approximation we can simplify the differential cross-section given by the Klein–Nishina Eq. (1) to (Rybicki and Lightman, 1985)

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}r_0^2\left(1 - \cos^2(\theta)\right),\qquad(7)$$

and the total cross-section is then reduced to

$$\sigma_T = \frac{8\pi}{3}r_0^2.\qquad(8)$$

The $\text{cdf}_{TH}(\theta)$ can be obtained by integration of the Eq. (7) and it has form

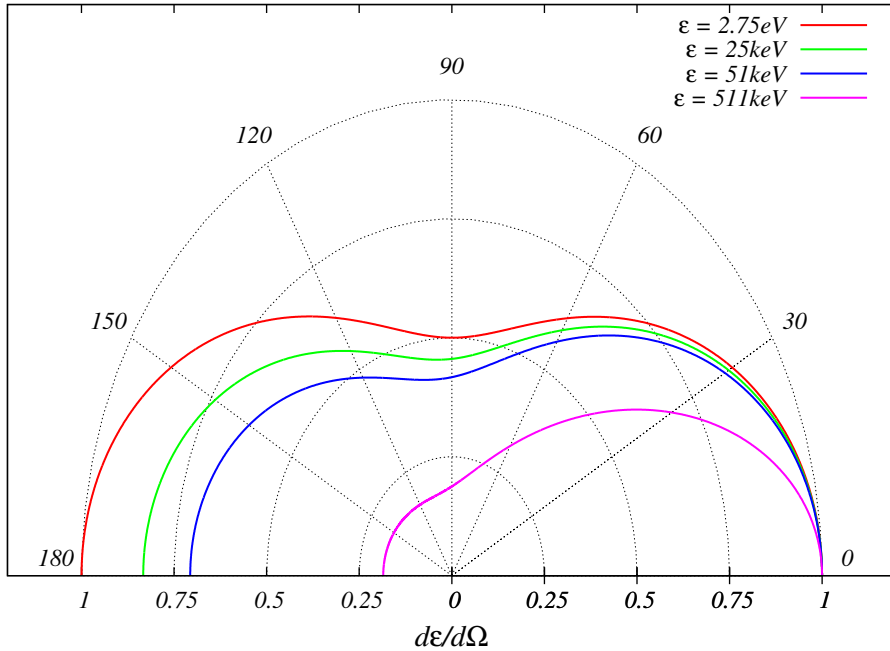$$\text{cdf}_{TH}(\theta) = \frac{1}{8}r_0^2\left(6\theta + \sin(2\theta)\right).\qquad(9)$$

Figure 1. Differential cross-section $d\epsilon/d\Omega$ of Compton scattering for low energy photons as it depends on scattering angle. The cross-sections are normalized. Chosen photon energies demonstrate deviation of $d\epsilon/d\Omega$ with increasing photon energy. Differential cross-section for photons with energy above $\epsilon = 51$ keV starts to deviate from Thomson limit (photons with $\epsilon = 2.75$ eV).

Implementation in the code

As with Compton scattering the library contains similar functions for Thomson approximation. To get differential cross-section (7) call of function `TH_diffcr` is appropriate. Thomson total cross-section is stored at variable `TH_totcr` since it is independent on incident photon energy. To get the value of the $\text{cdf}_{TH}(\theta)$ one must call the function `TH_cdf_value`. However since we do not have direct expression for inverse $\text{cdf}_{TH}(\theta)$, the Thomson approximation is not useful in a sense of performance. In other words using Thomson approximation for evaluation of low energy photons we would not gain any increase in performance.

2.3 Inverse Compton Scattering

If we restrict ourselves just to scattering particle at rest we are confined to Compton scattering frame where photons can only loose energy. To increase energy of the scattered photons we need to take into account motion of the scattering particle as well. Since we are able to calculate Compton scattering only in the frame where the scattering particle is at rest we must transform photon's momentum by Lorentz transformation into this rest frame first. This transformation involves two effects: The first effect is relativistic aberration or beaming

effect. This effect changes the angle α between scattering particle's velocity and incident photon direction. This transformation reads (Rybicki and Lightman, 1985)

$$\cos(\bar{\alpha}) = \frac{\cos(\alpha) + \beta}{1 + \beta\cos(\alpha)}, \tag{10}$$

where $\beta = |v_e|/c$ and $|v_e|$ is electron velocity. This effect is applied to both incident and radiated photons.

The second phenomenon is the Doppler effect which modifies photon frequency thus causes increase or decrease of its energy as measured by observer comoving with electron. The energy of the interacting photon is transformed as follows (Rybicki and Lightman, 1985)

$$\bar{\epsilon}_i = \epsilon_i \gamma \left(1 - \beta\cos(\alpha)\right), \tag{11}$$

where again $\beta = |v_e|/c$. This transformation must be performed before as well as after scattering took place.

3   ELECTRON VELOCITY

3.1   Maxwell–Boltzmann Distribution

Maxwell–Boltzmann distribution gives distribution of velocities of particles of ideal gas. We assume point-like, non-relativistic particles with negligible inter-particle forces. Many gases in astrophysics behave as ideal gas or they are similar to it. In Compton scattering scheme we are mostly dealing with rarefied real gasses. For these, at ordinary temperatures, the Maxwell–Boltzmann distribution is a good approximation.

The probability of particle having magnitude of velocity p within a gas with temperature T is given as (Bradt, 2014)

$$\text{pdf}_{\text{MB}}(v) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi v^2 \exp\left(-\frac{mv^2}{2kT}\right), \tag{12}$$

where k is Boltzmann constant $k = 8.61 \times 10^{-5}$ eV/K and m is mass of the gas particle (in this case electrons $m_e = 9.11 \times 10^{-31}$ kg). To acquire cumulative distribution function $\text{cdf}_{\text{MB}}(v)$ we must integrate (12)

$$\text{cdf}_{\text{MB}}(v) = \text{erf}\left(\sqrt{\frac{mv^2}{2kT}}\right) - \sqrt{\frac{2mv^2}{\pi kT}} \exp\left(\frac{mv^2}{2kT}\right), \tag{13}$$

where $\text{erf}(x)$ is Error function.

Implementation in the code

Maxwell–Bolzmann distribution is implemented in these routines: `MB_pdf` returns value of $\text{pdf}_{\text{MB}}(v)$ Eq. (12), `MB_cdf` gives $\text{cdf}_{\text{MB}}(v)$ Eq. (13). The function for random electron

speed is called `Random_num_icdf_bisection_MB` and it returns electron speed sampled from Maxwell–Boltzmann distribution. To evaluate $\mathrm{cdf}_{MB}(v)$ we are using GSL library implementation of Error function $\mathrm{erf}(x)$ by calling `gsl_sf_erf()`.

If the temperatures throughout the simulation do not exceed $T_B = 2 \times 10^8$ K the Maxwell–Boltzmann distribution can be used reasonably well. However if the temperature $T > T_B$ we recommend using Maxwell–Jüttner distribution for whole computation.

3.2   Maxwell–Jüttner Distribution

The Maxwell–Jüttner distribution is a generalization of the Maxwell–Boltzmann distribution for ideal non-interacting gas. For low temperatures T and in limit of small velocities this distribution becomes identical with the Maxwell–Boltzmann distribution.

Probability distribution for γ of the electrons within the gas with temperature T such that kT approaches or exceeds mc^2 is given by (Kershaw et al., 1986)

$$f(\gamma) = \frac{\gamma^2 \beta}{\tau K_2(1/\tau)} \exp -\frac{\gamma}{\tau} , \tag{14}$$

where $\beta = v/c$, $\tau = kT/mc^2$, K_2 is Bessel function of the second kind and c is speed of light.

Integral through all velocities must be

$$\int_{-\infty}^{\infty} f(\gamma) = 1 . \tag{15}$$

Behaviour of the distribution for low temperatures can be seen in the Fig. 2.

Implementation in the code

In the code we implement the distribution using logarithmic expression $\ln f(\gamma)$. This is advantageous because we can express Bessel function K_2 in its logarithmic form thus reducing possible errors due to round-off error. For calculating Bessel function we are using GSL library by calling function `gsl_sf_bessel_lnKnu()`. After we got value $\ln f(\gamma)$ we return $\exp(\ln f(\gamma))$.

Random number with Maxwell–Jüttner distribution

Implementation of random number generation, which produces random numbers with Maxwell–Jüttner distribution is similar to the technique described in Section 4.2. There is slight modification of the binary search starting position which is determined by the function `get_points_MJ()`. This function returns approximation of the peak of the distribution and end point of the distribution (which is a point where $f(\gamma) < 10^{-30}$). The aim is to decrease searching time and number of evaluations of the $\mathrm{cdf}(x)$ (which involves integrals) by setting middle point to the peak thus near most probable random value.

Cut-off Temperature

From the Fig. 2 we can see that for temperatures $T < 2 \times 10^8$ K the distribution has its maximum very near $\gamma = 1$. Thus no relativistic effects are noticeable. Putting cut off temperature to $T_{cut} = 2 \times 10^8$ K is reasonable.
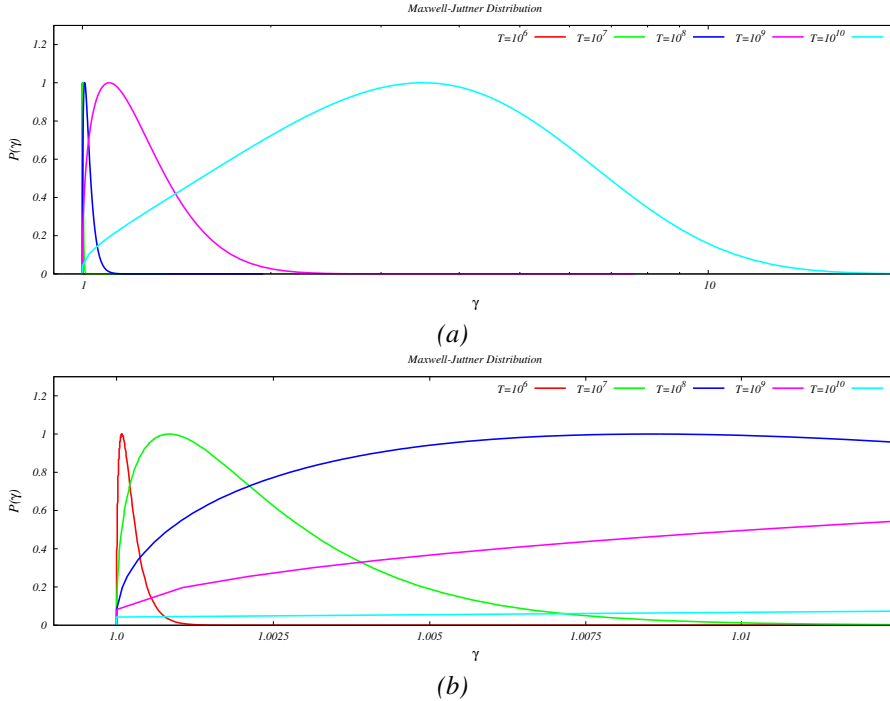

(a)

(b)

Figure 2. Maxwell–Jüttner distribution for different temperatures. Probability $P(\gamma)$ is normalized to unity.

4 NUMERICAL METHODS

Our simulation, in current state, is intended to follow single photons by using Monte Carlo method. The Monte Carlo method heavily depends on random numbers and thus good random number generator is needed for accurate results.

4.1 Random Number Generators

On computer using algorithms it is very hard if not impossible to get truly random unbiased, uncorrelated random numbers with uniform distributions in multiple dimensions. When using computer we are using a pseudo-random numbers produced by the pseudo-random number generators like `rand` in standard C. However some generators are better then others. The 'good' random number generator should pass number of theoretical and empirical tests. More can by found in (L'Ecuyer and Simard, 2007).

For our Monte Carlo simulation we choose to use `GSL` library random number generator `MT19937`. This generator has unusually long period of $P = 2^{19937} - 1$ numbers. This algorithm has been developed with special attention to the most significant bits. This property makes it especially well suited for Monte Carlo simulations (Matsumoto and Nishimura, 1998). With performance comparable to the standard C `rand` it is ideal pseudo-random number generator for our needs. It also performed well in tests conducted by (L'Ecuyer and Simard, 2007).

4.2   Random Numbers with Distribution

Standard random number generator produces uniformly distributed random numbers in range (0, 1). To obtain random numbers with desired custom distribution we must project this range onto some other which is defined by $\text{cdf}(x)$. For this projection we need to find an inverse cumulative distribution function $\text{cdf}(x)^{-1}$ of our custom distribution. To check if our custom distribution of random numbers does agree with $\text{cdf}(x)$ we have used Kolmogorov–Smirnov test for random number distribution (Wall and Jenkins, 2003).

Inverse cdf method

Assuming we have probability density function $\text{pdf}(x)$ with property

$$\int_{-\infty}^{\infty} \text{pdf}(x')\, \mathrm{d}x' = 1\,, \tag{16}$$

we can construct cumulative distribution function $\text{cdf}(x)$ given as

$$\text{cdf}(x) = \int_{-\infty}^{x} \text{pdf}(x')\, \mathrm{d}x'\,. \tag{17}$$

Taking into consideration the Eq. (16) we can see that $\text{cdf}(x) \in [0, 1]$. To generate random numbers with distribution given by $\text{pdf}(x)$ we need to construct inverse cumulative distribution function $\text{cdf}(x)^{-1}$ and project generated random numbers in interval (0, 1) by the $\text{cdf}(x)^{-1}$ to get random number with desired custom distribution. If we cannot find $\text{cdf}^{-1}(x)$ than we have to find appropriate function value by using root-finding algorithm. Since $\text{cdf}(x)$ is strictly increasing in the interval (0, 1) we can apply bisection to find the value of the $\text{cdf}^{-1}(x)$.

5   IMPLEMENTATION

5.1   Structures and constants

The COSMOC library uses these classes:

- `kn_par` class is directly used by user and it holds all variables connected with the scattering of the photon. For example it holds energy of the incident photon `kn_par::nu_i`, energy of the scattered photon `kn_par::nu_f`, scattering angles `kn_par::theta_f` and `kn_par::phi_f`. These are variables most likely to be accessed by the user.
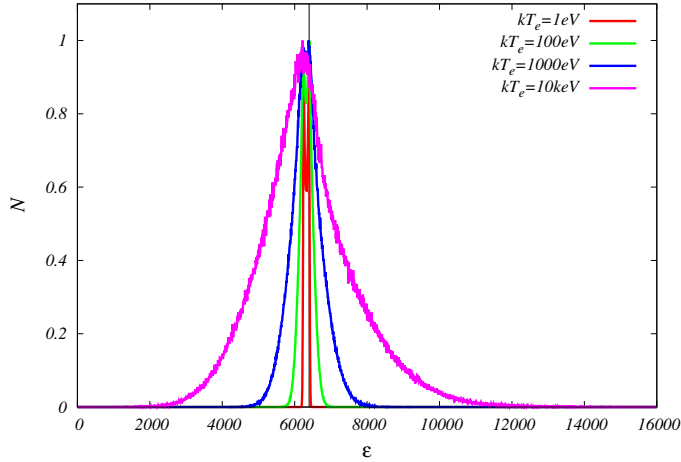- `prop`, `approx` and `Max_dis_int` are internal classes and user does not need to interact with them.

Figure 3. Broadening of iron spectral line with initial energy $\nu = 6400\,\text{eV}$. On x axis we see energy of the scattered photon, y axis shows normalized count. The scattering is performed on electrons with different temperatures, where k is Boltzmann constant and T_e is electron temperature. Temperatures are distinguished by different colours.

5.2 Scattering

The whole process of scattering is performed by function `scatter_EDiE`, which then makes use of other internal functions of COSMOC library. These internal functions are accessible by user. Whole library as of now has a form of includable `.h` and `.cpp` file and it is not en-capsuled into a class. The declaration of function `scatter` is following:

```
void scatter_EDiE(
    kn_par *par – information about incident photon,
    double eT – temperature of the gas,
    approx *mj_app – internal class which must be initiated at the beginning of the code,
    int mj_size – size of mj_app,
    gsl_rng *rnd – GSL library handle for random numbers
    gsl_integration_workspace *w – GSL library handle for integration,
    int force_relativistic=0 – optional switch to force relativistic treatment
).
```

The procedure `scatter_EDiE` works in three modes, which mode is triggered depends on temperature of the gas. For temperatures $T > 2.0 \times 10^8$ K the relativistic treatment is used. This includes beaming effect Eq. (10) and Doppler effect Eq. (11). For electron velocities the Maxwell–Jüttner distribution is used.

The second mode is for temperatures $300\,\text{K} < T < 2.0 \times 10^8$ K. In this mode Maxwell–Boltzmann distribution is used and only Doppler effect is taken into account.

Last mode is for stationary electrons for temperatures below $T = 300$ K, where only Compton scattering without any additional effects is performed.

The effect of Doppler shift can be seen on spectral line broadening, which is shown in the Fig. 3. The figure shows broadening of iron $\nu = 6.4\,\text{keV}$ spectral line.

SUMMARY

The COSMOC library simulates Compton scattering by following single photon by Monte Carlo method. It includes Compton as well as inverse Compton scattering. We have implemented Maxwell–Boltzmann distribution of electron velocities and it's relativistic version the Maxwell–Jüttner distribution. The random number generator used is `MT19937`. The accuracy of generated distribution (Klein–Nishina, Maxwell–Boltzmann, Maxwell–Jüttner) were tested by using Kolmogorov–Smirnov test. The functions in COSMOC library can also be used separately.

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