Single Compton scattering module for particle-in-cell codes

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We detail the implementation of a novel numerical tool, coded within the framework of QED-OSIRIS, which allows the self-consistent study of high frequency radiation within a plasma.

1. Introduction

Computer simulations for kinetic plasma processes are of core interest for a variety of scenarios, ranging from astrophysics to laboratory experiments. Two different approaches exist to simulate kinetic effects: Vlasov codes that require a fine discretization of the plasma phase-space, and particle-in-cell (PIC) codes that provides a numerical solution to the Klimontovich equation with macro-particles. Particle-in-cell simulations (Evans & Harlow 1957; Dawson 1983; Bird 1989; Birn & Langdon 1991; Hockney & Eastwood 1988), which pioneered the study of collisionless plasmas, have computational advantages compared to Vlasov codes and are nowadays widely used for studying fundamental plasma processes. To study astrophysical environments and model laboratory experiments where the plasma dynamics are affected by quantum processes, the standard PIC loop can be enriched with modules that account for various Quantum Electrodynamics (QED) cross sections. These modules are based on Monte Carlo techniques due to the inherent stochasticity of QED processes. The coupling of QED Monte Carlo modules to the PIC loop represent a unique numerical tool where the feedback of the various quantum processes onto the plasma dynamics can be studied from first principles. For example, the inclusion of nonlinear Compton scattering and multi-photon Breit-Wheeler pair production are essential to simulate the interaction of matter with ultra intense electromagnetic fields (Nerush et al. 2011; Vranic et al. 2014; Blackburn et al. 2014; Vranic et al. 2016b; Lobet et al. 2016; Grismayer et al. 2016; Vranic et al. 2016a; Jirka et al. 2016; Grismayer et al. 2017). In nonlinear Compton scattering an electron interacts with multiple real photons in a coherent state. This photons are thus represented as a classical electromagnetic wave whose wavelength is resolved by the PIC grid. The result of nonlinear Compton events is the discrete emission by leptons of high energy photons, whose frequency can not be captured by the grid, and are represented as a particle-like photons in the QED-PIC code (Gonoskov et al. 2015). These high energy photons are usually considered as incoherent (their respective phase is random) and possess wavelengths considerably smaller than the average inter-particle distance of the plasma. They perceive the plasma as a rarefied gas where the leading photon - electron (positron) interaction mechanism is single Compton scattering (Compton 1923).

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The collision of these high energy photons with the plasma electrons explain the saturation properties of cyclotron radiation masers (Dreicer 1964), the relaxation to thermal equilibrium of a photon-electron gas (Kompaneets 1957; Pevzner 1968), or the Comptonisation of the microwave background (Sunyaev & Zel’dovich 1980). In these seminal results, the plasma is considered a gas of free electrons and its collective behaviour is neglected. Frederiksen (Frederiksen et al. 2008) and more recently the Authors (Del Gaudio et al. 2015) have shown that bursts of hard X-rays can indeed couple to the collective plasma dynamics via incoherent Compton scattering events and drive plasma waves. Such phenomena can be studied numerically by coupling a Monte Carlo Compton module to the PIC loop (Haugbølle 2005; Haugbølle et al. 2013).

The implementation of binary collisions in PIC codes is extensively discussed in the literature, with main focus on Coulomb collisions (Takizuka & Abe 1977; Wilson et al. 1992; Miller & Combi 1994; Vahedi & Surendra 1995; Nanbu 1997; Larson 2003; Kawamura & Birdsall 2005; Sherlock 2008). The usual implementation relies on the approximation of small cumulative scattering angles (Takizuka & Abe 1977; Miller & Combi 1994; Nanbu 1997), which allows to relax the simulation time step that is not bound to resolve the collision frequency. This improves considerably the computational performance, but neglects the effect of large angle collisions. Recently, Turrel (Turrell et al. 2015) and Higginson (Higginson 2017) included the effect of large angle collisions. Their technique is based on the separation of small angle collisions from large angle ones defining a cut-off angle that identifies the occurrence of one or the other. The cut-off angle angle is imposed according to the impact parameter of the colliding particles. In the case of Compton scattering an implementation based on small cumulative collisions is not possible, as the scattering angle ranges within $\theta \in [0, \pi]$ with comparable probability in the Thomson regime. In the Compton regime instead, the most likely interaction occurs for large scattering angles. The differential cross section for Compton scattering is derived for initial and final asymptotic electron and photon states, which implies neglecting the extent of the interaction in space. Therefore the definition of an impact parameter in the single Compton scattering theory is meaningless. We are bound to account for one scattering at a time in the implementation of single Compton collisions.

In this article we describe in details the implementation of a single Compton scattering collision module for particle-in-cell codes. It relies on first principles (the Klein-Nishina (Klein & Nishina 1923) cross section is employed with no approximations) and allows a self-consistent treatment of the high frequency radiation coupling with the plasma dynamics. In section 2 we review briefly the basic theory for Compton scattering with particular attention to the Lorentz invariant quantities that the code must enforce for reproducing the correct scattering rates in the collision at relativistic energies (Peano et al. 2009). The section 3 is devoted to the implementation of our collision procedure. In Section 4 we benchmark our code against problems for which exact analytical solution or formulation exist, namely the scattering photon spectrum of a relativistic charge (Blumenthal & Gould 1970), and the Kompaneets equation (Kompaneets 1957). Finally, in Section 5 we comment on the computational cost that our module introduces as compared to a standard PIC loop.
2. Compton scattering

Single Compton scattering is the inelastic collision between a photon and an electron (Compton 1923). It is the generalization of Thomson scattering (Thomson 1906), for any value of the incident photon of energy $\hbar \omega$ in the electron proper frame of reference. By applying energy and momentum conservation in the electron rest frame,

\begin{align*}
\hbar \omega + mc^2 &= \hbar \omega' + \gamma' mc^2, \\
\hbar k &= \hbar k' + p',
\end{align*}

(2.1)
(2.2)

where $\gamma' = \sqrt{1 + p'^2/m^2 c^2}$, and $\omega = ck$, one can derive the photon frequency shift over one collision

$$\frac{\omega'}{\omega} = \frac{mc^2}{mc^2 + \hbar \omega (1 - \cos \theta)},$$

(2.3)

where $\omega$ ($\omega'$) is the absorbed (emitted) frequency, and $\theta$ is the scattering angle. For $\hbar \omega \ll mc^2$ one recovers the Thomson limit $\omega' \simeq \omega$. However, when the incident photon energy approaches and exceeds the electron rest mass energy $\hbar \omega \gtrsim mc^2$, the energy transfer becomes relevant. For $\hbar \omega \gg mc^2$, at $\theta \simeq -\pi$, the photon cedes to the electron up to half its energy $\hbar (\omega - \omega') \simeq \hbar \omega/2$. The classical theory of radiation explains Thomson scattering in terms of plane wave absorption and consequent dipole radiation from the oscillating charge (Landau 2013; Jackson 2007), but does not predict Compton scattering, which is of purely quantum nature.

2.1. Klein-Nishina cross section

In the rest frame of an electron, the single Compton scattering probability is determined by the Klein-Nishina differential (in solid angle $\Omega$) cross section (Klein & Nishina 1923; Feynman 1998), which for unpolarised photons reads

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2} \left( \frac{\omega'}{\omega} \right)^2 \left( \frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \sin^2 \theta \right),$$

(2.4)

where $r_e = e^2/mc^2$ is the classical electron radius. By combining Eq.(2.3) for $\cos \theta$ and Eq.(2.4), an integration over the solid angle $d\Omega = \sin \theta d\theta d\phi$ ($\phi$ is the symmetry angle around the direction of the incoming photon) gives the total cross section

$$\sigma(\epsilon) = \frac{\pi r_e^2}{\epsilon} \left[ \left( 1 - \frac{2}{\epsilon} - \frac{2}{\epsilon^2} \right) \log(1 + 2\epsilon) + \frac{1}{2} + \frac{4}{\epsilon} - \frac{1}{2(1 + 2\epsilon)^2} \right],$$

(2.5)

where $\epsilon = \hbar \omega/mc^2$. In the limit for low photon energies

$$\lim_{\epsilon \to 0} \sigma(\epsilon) = \sigma_T$$

the Thomson cross section is recovered. For high photon energies $\epsilon \gg 1$ the cross section has the limiting expression

$$\lim_{\epsilon \gg 1} \sigma(\epsilon) = \frac{3}{4} \frac{\sigma_T}{\epsilon},$$

and decreases with respect to the incident photon energy.

2.2. Relativistic kinematics and Lorentz invariants

We consider a relativistic electron which propagates along the $z$ coordinate at a velocity $\beta c$ and scatters with a photon with an incident angle $\phi$ in the laboratory frame, see Fig. 1. In the electron proper frame of reference $O$, the incident angle is modified by relativistic
effects. In the frame $O$ the incident photon is confined within a small cone

$$\tan \phi_O = \frac{\sin \phi}{\gamma (\cos \phi - \beta)} \quad (2.6)$$

of aperture $1/\gamma$. The photon energy in the frame $O$ reads

$$\epsilon_O = \gamma \epsilon (1 - \beta \cos \phi). \quad (2.7)$$

It varies in the range $\epsilon_O \in [\epsilon/2\gamma, 2\epsilon/\gamma]$ according to the incident angle $\phi$. In the $O$ frame, the photon energy after scattering obeys Eq. (2.3) and in the laboratory frame reads

$$\epsilon' = \gamma \epsilon' O [1 + \beta \cos (\pi - \theta_O - \phi_O)] \simeq \gamma \epsilon'_O (1 - \cos \theta_O), \quad (2.8)$$

due to the Lorentz transformation, where $\beta \simeq 1$ and $\phi_O \sim 1/\gamma$. In the Thomson regime, $\omega'_O \simeq \omega_O$ and the maximum energy achieved over one collision is $\epsilon' \simeq 4\gamma^2 \epsilon$, for $\phi \simeq \pi$ and $\theta_O \simeq \pi$. In the extreme Klein-Nishina limit, the maximum energy achieved over one collision can be obtained by combining Eqs. (2.3), (2.7), and (2.8), and reads $\epsilon' \simeq \gamma$.

If we now consider the scattering between photons, with distribution function $f_\omega$, and electrons, with distribution function $f_e$. Within a portion of space-time $dxdt$, the number of collisions is a Lorentz invariant quantity (Groot et al. 1980) that is given by

$$N = \sigma(p, k) c f_\omega dk f_e dp dx dt. \quad (2.9)$$

In general, the cross section $\sigma(p, k)$ depends on the electron momentum $p$, and on the photon wavevector $k$. As the space-time element $dxdt$, the distribution functions $f_\omega$ and $f_e$, and the speed of light $c$ are Lorentz invariant therefore $\sigma(p, k)dkdp$ is also Lorentz invariant (Landau 2013). This invariance allows to obtain the cross section in any inertial frame ($\gamma = \sqrt{1 + p^2/m^2c^4}$, $\epsilon = h|k|/mc^2$). Knowing the cross section in the electron proper frame of reference ($\gamma_O = 1$, $\epsilon_O = \gamma \epsilon = h\epsilon |k|/m^2c^2$)

$$\sigma(p, k)dkdp = \sigma(\omega_O)dk_0d\epsilon_O, \quad (2.10)$$

we finally obtain

$$\sigma(p, k) = \sigma(\epsilon_O) \frac{\epsilon_O}{\gamma \epsilon}, \quad (2.11)$$

since $dk/\epsilon$ and $dp/\gamma$ are Lorentz invariants (Landau 2013).

3. Single Compton scattering algorithm

The implementation of single Compton scattering in a PIC code must not only recover the correct microphysics of the process (frequency shift, angle, momentum recoil)
Figure 2. Schematic of the Compton scattering algorithm. It follows three steps: i) the macro-particles are binned into collision cells $\Delta x$, ii) the probability $P_{i,j}$ of interaction within $\Delta x \Delta t$ is computed and scattering macro-particles are chosen using the no-time-counter method, iii) the momenta of the scattering macro-particles are updated.

but must preserve the invariant number of collisions to obtain the correct scattering rates (Peano et al. 2009). The implementation follows naturally as each macro-particle represents an ensemble of real particles close in space and momentum. The weight $q$ of each macro-particle relates to the number of real particles within, thus each macro-particle samples a portion of the distribution function of real particles. Figure 2 outlines our implementation that follows three steps:

- binning of the macro-particles into collision cells $\Delta x$,
- pairing of the colliding macro-particles according to their probability $P_{i,j}$ of interaction within $\Delta x \Delta t$,
- update of the momenta of the scattering macro-particles.

3.1. Macro-particles binning

The binning of macro-particles in collision cells can naturally use the single PIC cell as the smallest binning volume. The size of a PIC cell is also the smallest scale over which the self-consistent plasma collective fields are computed. For this reason, the collision cells are usually set equal to the pic cells. Macro-photons and macro-electrons are binned in the collision cells and sorted such that we identify the indexes of macro-electrons and macro-photons within each collision cell.

3.2. Pairing

For each collision cell, we pair the scattering couples and add them to a scattering list using the no-time-counter method (NTC) (Bird 1989; Abe 1993). The NTC method is
one of the most popular Monte Carlo schemes for collision procedures. Developed three
decades ago (Bird 1989), it provides an undeniable cost reduction for the sampling of
a discrete probability distribution function. We detail the NTC algorithm applied to
single Compton scattering in the following. We consider a collision cell containing $N_\omega$
macro-photons and $N_e$ macro-electrons. A conservative upper-bound to the maximum
probability of any macro-particle to collide within $\Delta t$ is

$$P_{\text{max}} = 2\sigma_T c \Delta t \max[q^i_e, q^j_\omega]$$  (3.1)

where $\max[q^i_e, q^j_\omega]$ is the largest weight with units of a density among all macro-particles
in the collision cell ($i \in [1, N_e]$ macro-electrons and $j \in [1, N_\omega]$ macro-photons). The factor 2 appears conservatively as a consequence of the relativistic transformation of the
cross section $\sigma = \sigma_{T,O} \epsilon_O / \gamma \epsilon$, where $\max(\epsilon_O) = 2 \gamma \epsilon$. The maximum number of macro-
particles that can scatter $N_{\text{max}}$ is given by the maximum probability $P_{\text{max}}$ times the
number of all the possible unsorted pairing combinations $N_e N_\omega$ (potential scatterings)
of the macro-photons with the macro-electrons. It reads

$$N_{\text{max}} = P_{\text{max}} N_e N_\omega.$$  (3.2)

The number $N_{\text{max}}$ is usually not an integer and is rounded to the next or previous
integer by a Monte Carlo sampling of the residue. This procedure preserves statistically
the correct number of collisions within $\Delta x \Delta t$, thus it reproduces the correct rates. We
randomly pair $N_{\text{max}}$ macro-photons and $N_{\text{max}}$ macro-electrons. This is obtained in two
steps: i) a random sorting of the macro-photons and of the macro electrons (Knuth
shuffle) ii) the selection of the first $N_{\text{max}}$ indexes. At this point, we have a short list of
$N_{\text{max}}$ randomly paired macro-particles, which is only a subset of all potential scatterings
in the collision cell.

For each pair in the short list, a random number $\text{rnd} \in [0, 1]$ is rolled and compared
with the joint probability

$$P^{i,j} = \sigma(p^i, k^j) c \Delta t \max[q^i_e, q^j_\omega] / P_{\text{max}}$$  (3.3)

of scattering after having being selected within the $N_{\text{max}}$ pairs. To compute the cross
section $\sigma(p^i, k^j)$ we proceed as follows. The energy of the photon $k^j$ is Lorentz boosted
in the rest frame of the electron $p^i$

$$\epsilon^j_O = \gamma \epsilon^j - \hbar p^i \cdot k^j / m^2 c^2.$$  (3.4)

Then, the cross section $\sigma_C(\epsilon^j_O)$ is computed in this frame and boosted back in the
simulation frame using eq. 2.11. A macro-electron/macro-photon pair from the short list
is admitted to the scattering list based on a Rejection method (accepted if $\text{rnd} < P^{i,j}$).

### 3.3. Momentum update

For each pair in the scattering list, the momenta are updated according to the Compton
closest frequency shift and momentum recoil. The macro-photon four-wavevector $K = (\epsilon, \hbar k / mc)$
is Lorentz boosted in the electron, of momentum $p$, rest frame as $K_O = L(p) K$, where the boost matrix is

$$L(p) = \left[ \begin{array}{cc} \gamma & -p/mc \\ -p^T/mc & I + p^T p / m^2 c^2 (1 + \gamma) \end{array} \right],$$  (3.5)

and $I$ the $3 \times 3$ identity matrix. In the frame $O$, we identify the unit vector along the
photon propagation direction $\hat{k}_0$ which defines the symmetry axis for the scattering. We
define an orthonormal unit vector base $\hat{e}_1 = \hat{k}_0, \hat{e}_2 \perp \hat{e}_1, \hat{e}_3 = \hat{e}_1 \times \hat{e}_2$. The two scattering
angles $\theta$ and $\phi$ are then sampled, $\theta$ is the angle with respect to $\hat{e}_1$, and $\phi$ is the angle on the plane $\hat{e}_2, \hat{e}_3$. This latter, being the angle of rotational symmetry, is chosen randomly between 0 and $2\pi$. Instead the angle $\theta$ is obtained by the Inverse Transform Sampling method of the cumulative probability function. The probability distribution function (pdf) of the scattered macro-photon over the scattering angle $\mu = \cos \theta \in [1, -1]$ reads

$$\text{pdf}(\mu, \epsilon_O) = \frac{1}{\sigma(\epsilon_O)} \frac{d\sigma}{d\mu}, \quad \text{and} \quad \int_{1}^{-1} \frac{d\sigma}{d\mu} = \sigma(\epsilon_O)$$

(3.6)

with

$$\frac{d\sigma}{d\mu} = -\pi r_e^2 \left( \frac{1}{1 + \epsilon_O(1 - \mu)} \right)^2 \left( \frac{1}{1 + \epsilon_O(1 - \mu)} + \epsilon_O(1 - \mu) + \mu^2 \right)$$

(3.7)

The cumulative distribution function (cdf) is

$$\text{cdf}(\mu, \epsilon_O) = \frac{1}{\sigma(\epsilon_O)} \int_{1}^{\mu} \frac{d\sigma}{d\mu'} \int_{1}^{\mu} d\mu'$$

(3.8)

with

$$\int_{1}^{\mu} d\mu' \frac{d\sigma}{d\mu'} = \frac{\pi r_e^2}{\epsilon_O} \left\{ \left( 1 - \frac{2}{\epsilon_0} - \frac{2}{\epsilon_0^2} \right) \log \left[ 1 + \epsilon_O(1 - \mu) \right] \\
+ \frac{1 - \mu}{\epsilon_O} \left[ \frac{1 + 1 + 2 \epsilon_O}{1 + \epsilon_O(1 - \mu)} \right] \\
+ \frac{1}{2} \left[ 1 + \epsilon_O(1 - \mu) \right]^2 \right\}$$

(3.9)

In the inverse transform sampling method a random number is generated in the range $\text{rnd} \in [0,1]$, then $\mu = \text{cdf}^{-1}(\text{rnd}, \epsilon_O)$. Given the nonlinear dependence of the cdf on $\mu$, we use the bisection method to solve $\text{cdf}(\mu, \epsilon_O) - \text{rnd} = 0$. We preferred this method rather than a rejection method. The scattered photon energy is $\epsilon'_O$ given by eq. 2.3

$$\epsilon'_O = \frac{\epsilon_O}{1 + \epsilon_O(1 - \mu)}$$

(3.10)

and the scattered wavevector is

$$\frac{\hbar k'_O}{mc} = \epsilon'_O \left( \mu \hat{e}_1 + \sqrt{1 - \mu^2} \cos \phi \hat{e}_2 + \sqrt{1 - \mu^2} \sin \phi \hat{e}_3 \right)$$

(3.11)

We transform back to the simulation frame $\mathcal{K}'_O = (\epsilon'_O, \hbar k'_O/mc)$ simply as $\mathcal{K}' = \mathbb{L}(-\mathbf{p})\mathcal{K}_O$, and by conservation of momentum the scattered electron has a new momentum $\mathbf{p}' = \mathbf{p} + \hbar(\mathbf{k} - \mathbf{k}')$.

3.4. Note on macro-particles with difference in weight

In PIC codes, it is unlikely that two scattering particle possess exactly the same weight. This issue has already been addressed by [Haugbølle 2005] and relies on the splitting of the scattering macro-particles. Here, we address this problem similarly but only the largest weight macro-particle is split before scattering. We briefly recall the main steps of this procedure:

- Identify the two scattering macro-particles of weight $q'_e$ and $q'_\omega$, and select the largest weight between the two: $\max[q'_e, q'_\omega]$
- Create a new particle of weight equal to $\min[q'_e, q'_\omega]$
- The two macro-particles of equal weight $\min[q'_e, q'_\omega]$ are now paired and can Compton scattered as described before
- reassign to the split macro-particle the weight $\max[q'_e, q'_\omega] - \min[q'_e, q'_\omega]$
4. Benchmarks

In order to benchmark our algorithm, we choose two problems that possess exact analytical solution:

- the inverse Compton spectra produced by an electron scattering with an isotropic photon gas (Blumenthal & Gould 1970),
- the relaxation to thermal equilibrium of a photon gas by Compton collisions with a thermal electron gas of fixed non-relativistic temperature, Kompaneets equation (Kompaneets 1957).

4.1. Inverse Compton spectra

Blumenthal and Gould derived the inverse Compton spectra produced by the collision of a relativistic electron, $\gamma \gg 1$, with an isotropic gas of photons (Blumenthal & Gould 1970). If the photon gas is isotropic in the laboratory frame, it appears beamed at a small angle $\sim 1/\gamma$ in the proper frame $O$ of reference of an incident relativistic electron $\gamma \gg 1$, as shown by Eq. (2.6). The Compton scattering differential rate in the laboratory frame relates to the one in the frame $O$ as

$$\frac{dN}{dt d\epsilon} = \int d\epsilon_O \int d\Omega_O \frac{dN}{dt_O d\epsilon_O d\Omega_O} \frac{dt_O}{dt} \frac{d\epsilon_O}{d\epsilon'}.$$  \hspace{1cm} (4.1)

The time interval in the frame $O$ is $dt_O = dt/\gamma$, and the energy transforms according to Eq. (2.8) as $d\epsilon' \simeq \gamma(1 - \cos \theta_O)d\epsilon_O$. The Compton scattering differential rate in the frame $O$ is

$$\frac{dN}{dt_O d\epsilon_O d\Omega_O d\epsilon'_O} = c \frac{d\sigma(\epsilon_O)}{d\Omega_O} \delta(\epsilon' - \epsilon_O) \frac{dn_O}{d\epsilon_O},$$  \hspace{1cm} (4.2)

Here the $d\sigma(\epsilon_O)/d\Omega_O$ is the Klein-Nishina cross section. The photon density spectrum $dn_O/d\epsilon_O$ in the $O$ frame can be related with the isotropic differential photon density in the laboratory frame by the Lorentz invariance of the ratio $dn/\epsilon$.

$$\frac{1}{\epsilon_O} \frac{dn_O}{d\epsilon_O} = \frac{1}{\epsilon} \frac{dn}{d\epsilon}.$$  \hspace{1cm} (4.3)
The isotropic differential photon density in the laboratory frame reads $dn = \frac{1}{2} n(\epsilon) d\epsilon \cos \phi$, where $n(\epsilon)$ is the density of photons of a given energy $\epsilon$. According to Eq. (2.7), the incident angle in the laboratory frame results in a change in the photon energy in the $O$ frame as $|d\epsilon_O/d\cos \phi| \simeq \gamma\epsilon$. One thus obtain from Eq. (4.3)

$$\frac{d n_O}{d \epsilon_O} = \frac{\epsilon_O}{2\gamma \epsilon^2} n(\epsilon).$$ (4.4)

By combining Eqs. (4.4) and (4.2) with Eq. (4.1), and integration, the Compton scattering differential rate reads (Blumenthal & Gould 1970)

$$\frac{dN}{dtd\epsilon'} = \frac{3\sigma_T c n(\epsilon)}{4\gamma \epsilon} f(\Gamma, \epsilon'),$$ (4.5)

where $\epsilon' = \epsilon'/\epsilon'_{\text{max}}$ is the scattered photon energy normalised to its maximum $\epsilon'_{\text{max}} = \gamma\Gamma/(1 + \Gamma)$. The parameter $\Gamma = 4\epsilon\gamma$ relates to the energy of the scattering photons in the electron rest frame and distinguishes two regimes: i) Thomson limit $\Gamma \ll 1$ and ii) extreme Klein-Nishina limit $\Gamma \gg 1$. The scattered photon distribution function reads

$$f(\Gamma, \epsilon') = 2q \log q + (1 + 2q)(1 - q) + \frac{1}{2} \frac{\Gamma^2 q^2}{1 + T q}(1 - q)$$ (4.6)

where $q = \epsilon'/[1 + \Gamma(1 - \epsilon')]$.

Figure 3 shows an excellent agreement between our simulations (dashed lines) and theory (solid lines) for $\Gamma = 0.1, 10, 100$. The scattered photon distribution function $f(\Gamma, \epsilon')$ is normalised $\int d\epsilon' f(\Gamma, \epsilon') = 1$. In our simulations, the photon gas is initialised with $1.5 \times 10^7$ macro-photons which mimic an emission line. All macro-photons have same energy and are propagating in random directions, uniformly distributed on a sphere in momentum space. We considered the interaction at different photon energies $\epsilon = 0.00025, 0.025, 0.25$. An equal number of macro-electrons are initialised at a Lorentz factor of $\gamma = 100$ collimated in one direction. The initialisation of this many macro-electrons is equivalent to simulating that many collisions with only one macro-electron at a time, but speeds up the benchmark. To avoid multiple scatterings the simulation runs for only one time step where about $1 \times 10^6$ macro-scatterings occur. The only constraint on $\Delta t$ is to be low enough such that $P_{\text{max}} < 1$, as multiple scatterings are not computed within a single time step.

### 4.2. Photon-electron gas equilibrium (Kompaneets equation)

Kompaneets addressed the thermodynamic equilibrium which establishes between photons and free electrons if their interaction is only mediated by Compton scattering events (Kompaneets 1957). He derived the partial differential equation that describes the temporal evolution of the photon occupation number $n$ resulting from the interaction with an electron gas of fixed thermal energy $k_B T$, $k_B$ is the Boltzmann constant. The full collision operator reads

$$\frac{\partial n}{\partial t} = c \int d\mathbf{p} d\sigma d\Omega \left[ f_e' n'(1 + n) - f_e n(1 + n') \right]$$ (4.7)

where $f_e = f_e(\gamma)$ and $f_e' = f_e(\gamma')$ refer to the electron energy distribution function evaluated at a Compton transition $\gamma mc^2 + \hbar \omega = \gamma' mc^2 + \hbar \omega'$. The evaluation of the photon occupation numbers $n = n(\omega)$ and $n' = n(\omega')$ follow the same definition. The $n^2$ terms account for the photon Bose-Einstein statistics where phenomena like stimulated scattering and superposition of states are considered. In the Thomson limit $\hbar \omega \ll mc^2$,
Figure 4. Time evolution of the photon distribution function $f(\xi)$ by the interaction with an electron gas of density $10^{18}$ cm$^{-3}$ at 5 keV temperature for times $y = 0$, 0.5, 1, 3. After $y = 3$ the photon distribution function resembles the Wien spectrum and does not evolve significantly. Simulations in dashed lines and solution of the linear Kompaneets equation in solid lines (Kompaneets 1957).

The energy exchange of one transition is small compared to the energy of the photon $\delta \omega = |\omega' - \omega| \ll \omega$. The energy exchange over one Compton event is

$$\delta \omega = \frac{\hbar(1 - \hat{k}' \cdot \hat{k})}{\gamma mc^2 + \hbar(1 - \hat{k}' \cdot \hat{k})} - \frac{\hbar (1 - \hat{k}' \cdot \hat{k})}{mc^2 (1 - \hat{k}' \cdot \hat{k})}.$$  

(4.8)

where $\hat{k} = k/k$ and $\hat{k}' = k'/k'$ are the unit vectors that identify the photon propagation direction before and after scattering. In such regime, the functions $f'_e$ and $n'$ can be expanded to second order in the small parameter $\delta \omega$ allowing the reduction of the full collision operator to a Fokker-Planck form that reads

$$\frac{\partial n}{\partial t} \approx \left[ \frac{\partial n}{\partial \xi} + n(1 + n) \right] \int d\mathbf{p} \frac{d\sigma}{d\Omega} f_e \frac{\hbar \delta \omega}{k_B T}$$

$$+ \left[ \frac{\partial^2 n}{\partial \xi^2} + (1 + n) \left( \frac{2 \partial n}{\partial \xi} + n \right) \right] \int d\mathbf{p} \frac{d\sigma}{d\Omega} f_e \left( \frac{\hbar \delta \omega}{k_B T} \right)^2,$$

(4.10)

where the electron distribution function is assumed to be Maxwellian, and $\xi = \hbar \omega / k_B T$ is the normalised energy. The expansion parameter $\delta \omega$ is small in the laboratory frame only if it is small also in the proper frame of each electron. This holds for non relativistic electron temperatures $k_B T \ll mc^2$. The two integrals in $\delta \omega$ and in $\delta \omega^2$ can be evaluated assuming the differential cross section in the Thomson limit

$$\frac{d\sigma}{d\Omega} = \frac{r^2}{2} (1 + \cos^2 \theta).$$

(4.11)
Then, the time evolution of the average occupation photon number $n$ reads (Kompaneets 1957)

$$\xi^2 \frac{\partial n}{\partial y} = \frac{\partial}{\partial \xi} \left[ \xi^4 \left( \frac{\partial n}{\partial \xi} + n + n^2 \right) \right].$$

(4.12)

where $y = t/t_C$ is the time normalised to $t_C = mc/\sigma_T n_e k_B T$, $n_e$ is the electron gas density. The time $t_C$ is the relaxation time of the process, such that a time $y = 3$ is a good estimate for the time at which the thermal equilibrium establishes.

In regimes where the photon occupation number is small, $n \ll 1$, the photon electron gas interaction is mediated by single Compton scattering events and the equation reduces to its linear form

$$\xi^2 \frac{\partial n}{\partial y} = \frac{\partial}{\partial \xi} \left[ \xi^4 \left( \frac{\partial n}{\partial \xi} + n \right) \right].$$

(4.13)

For convenience we work with the photon energy distribution function $f = \xi^2 n$ for which the linear Kompaneets equation reads

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial \xi} \left[ \xi^5 \frac{\partial f}{\partial \xi} + (\xi^2 - 2\xi) f \right].$$

(4.14)

Figure 4 shows the excellent agreement between our algorithm and the numerical solution of the linear Kompaneets equation obtained with a finite difference centred scheme. In our simulation, more than $10^5$ macro-photons are initialised to mimic an emission line at an average energy of $\bar{\xi} = \langle \xi \rangle = 0.2$. The emission line has a small energy spread of $\sigma^2_\xi = \langle \xi^2 - \bar{\xi}^2 \rangle = 0.1$, and the initial distribution

$$f(\xi, y = 0) \propto \exp \left[ -\frac{(\xi - \bar{\xi})^2}{2\sigma^2_\xi} \right]$$

(4.15)

is Maxwellian. As many macro-electrons follow a Maxwellian distribution at the given temperature (5 keV). They are set to free stream such that fluctuations of the electron density do not feed back on the particles through the collective field. Moreover, the electron recoil is here disabled as the electron equilibrium temperature is fixed, their distribution is assumed constant by Kompannets. After a time $y \gtrsim 3$, the photon energy distribution reaches equilibrium and does not evolve but only fluctuates around the Wien’s spectrum $f \propto \xi^2 \exp(-\xi)$, the correct equilibrium for the linear Kompaneets equation.

5. Algorithm performance

In this section we compare the computational cost of our Compton scattering algorithm with the standard PIC loop. The computational performances of our algorithm are usually dependent on the physical parameters of the particular simulated system. A thorough benchmark of its performance should then cover a variety of physical parameters of relevant case scenarios. In collisional plasmas, a typical benchmark of the performance of a collisional algorithm relies on the simulation of a thermal plasma with and without collision. Our choice for the comparison follows a similar criterion. We simulate in 1D a thermal plasma in equilibrium with a photon gas both at a temperature of 5 keV. The plasma density is $n_p = 10^{18}$ cm$^{-3}$ and the photon density is $n_\omega = 3 \times 10^{27}$ cm$^{-3}$, chosen such that the electron Compton collision frequency is a tenth of the plasma frequency $c\sigma_T n_\omega = \omega_p/10$. Figure 5 shows the initial equilibrium spectra for electrons (blue) and photons (red) function of the kinetic energy $W_k$. The electrons follow a Maxwell-
Figure 5. Initial equilibrium spectra for electrons (blue) and photons (red) function of the kinetic energy $W_k$. The electrons follow a Maxwell-Boltzmann distribution, theory in dashed $f \propto \sqrt{W_k} \exp(-W_k/k_BT)$. The photons follow a Wien distribution, theory in dashed $f \propto W_k^2 \exp(-W_k/k_BT)$. Simulation for $k_BT = 5 \text{ keV}$, $n_p = 10^{18} \text{ cm}^{-3}$, and $n_\omega = 3 \times 10^{27} \text{ cm}^{-3}$.

Figure 6. Time of a PIC loop per simulation particle with ($\times$) and without ($O$) Compton collisions as a function of the number of particles per cell (ppc). For a low number of ppc, the loop time is determined by the particle sorting routine (dependent also on the number of grid cells) used by the Compton module. For a high number of ppc, the scaling of our collision algorithm is proportional to the amount of simulated particles.
Boltzmann distribution, theory in dashed $f \propto \sqrt{W_k} \exp(-W_k/k_B T)$. The photons follow a Wien distribution, theory in dashed $f \propto W_k^2 \exp(-W_k/k_B T)$. The computational domain is $24 \, d_e$ long and divides into 240 cells. The time-step is $\Delta t = 0.099 \, \omega_p^{-1}$. Periodic boundary conditions are used. Figure 6 shows the time of a PIC loop per simulation particle with ($\times$) and without ($\bigcirc$) Compton collisions as a function of the number of particles per cell (ppc). For a low number of ppc, the loop time is determined by the particle sorting routine (dependent also on the number of grid cells) used by the Compton module. For a high number of ppc, the scaling of our collision algorithm is proportional to the amount of simulated particles.

6. Conclusions

We presented a collision algorithm which incorporates the effect of single Compton scattering from high frequency photons for particle-in-cell codes. This allows a self-consistent treatment of the high frequency radiation coupling with the plasma dynamics from first principles. The algorithm shows excellent agreement with respect to the benchmarks: scattering photon spectrum from the collision with relativistic electrons (Blumenthal & Gould 1970) and the relaxation to thermal equilibrium of a photon population with an electron gas (Kompaneets 1957). This framework is at the forefront for the numerical modelling of photon-plasma interaction and opens new and exciting opportunities in the numerical investigation of plasma phenomena.

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