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Monte Carlo simulation of Maxwell molecule interactions in space plasma

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Abstract A Maxwell molecule interactions model by the Monte Carlo method is proposed for space plasma simulations. The model describes a collision between a minor ion with a background neutral. As a result of a Maxwell molecule collisions, the magnitude of the relative velocity is unchanged but its direction is altered. However, the velocity of the center of gravity remains the same both in magnitude and direction before and after the collision. In the simulation, pairs of particles are generated at random, the changes in the velocities due to Maxwell molecule interactions are calculated.

Keywords Monte Carlo simulation, Maxwell-molecule interactions, space plasma.

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In dealing with gas mixtures, it is convenient to describe each species in the mixture by a separate velocity distribution function $f_s(\boldsymbol{r}_s, \boldsymbol{v}_s, t)$. The velocity distribution function is defined such that $f_s(\boldsymbol{r}_s, \boldsymbol{v}_s, t)\, d\boldsymbol{v}_s d\boldsymbol{r}_s$ represents the number of particles of species s which at time t, have velocities between $\boldsymbol{v}_s$ and $\boldsymbol{v}_s + d\boldsymbol{v}_s$ and positions between $\boldsymbol{r}_s$ and $\boldsymbol{r}_s + d\boldsymbol{r}_s$. The evolution in time of the $f_s(\boldsymbol{r}_s, \boldsymbol{v}_s, t)$ is determined by the net effect of collisions and the flow in phase space $(\boldsymbol{r}_s, \boldsymbol{v}_s)$ of particles under the influence of external forces (gravitational, electric, polarization, and magnetic). The mathematical description of this evolution is given by the well-known Boltzmann equation [1]

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v}_s \cdot \nabla f_s + \left[\boldsymbol{G} + \frac{e_s}{m_s}\left(\boldsymbol{E} + \frac{\boldsymbol{v}_s \times \boldsymbol{B}}{c}\right)\right] \cdot \nabla_{v_s} f_s = \left(\frac{\delta f_s}{\delta t}\right)_{coll}, \quad (1)$$

where $\boldsymbol{E}$ is the electric field, $\boldsymbol{B}$ is the magnetic field, $\partial/\partial t$ is the time derivative, ∇ is the coordinate space gradient, ∇_{v_s} is the velocity space gradient, c is the speed of light, and e_s and m_s are the charge and mass of species s. The quantity $(\delta f_s / \delta t)$ represents the rate of change of $f_s(\boldsymbol{r}_s, \boldsymbol{v}_s, t)$ in a given region of phase space $(\boldsymbol{r}, \boldsymbol{v})$ as a result of collisions. As far as the collision term is concerned, the appropriate expression for binary elastic collision between ions and neutrals is the Boltzmann collision integral [2]

$$\frac{\delta f_s}{\delta t} = \sum \int d\boldsymbol{v}_b d\Omega g_s \sigma_{st}(g_{sb}, \chi)\left[f_s' f_b' - f_s f_b\right], \quad (2)$$

where $d\boldsymbol{v}_b$ is the volume element in velocity space, $d\Omega$ is an element of solid angle in the center-of-mass reference frame, χ is the center-of-mass scattering angle, $\boldsymbol{g}_{sb}$ is the relative velocity of the colliding particles s and b, $\sigma_{st}(g_{sb}, \chi)$ is the differential scattering cross section, and the primes denote quantities evaluated after a collision. For partially ionized plasmas (Boltzmann's equation can be solved for each test species independently of the other species), there are essentially three collision terms that have been extensively used to describe the relevant collision processes (ion-ion Coulomb interactions, ion-neutral polarization interactions and ion-neutral resonant charge exchange interactions).

In this paper, however, our main concern is for ion-neutral collision processes dominated by the long-range polarization

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interaction [3]. With this so called Maxwell molecule interaction, the ion-neutral collision frequency is independent of velocity, and as a consequence, the calculation of ion velocity distribution function is significantly simplified. This interaction model is often used to simulate non-resonant ion-neutral interactions [4]. For this model, the differential scattering cross section $\sigma(g_{sb},\chi)$ is independent of scattering angle χ and inversely proportional to the relative speed g_{sb} *i.e.*

$$\sigma_{st}(g_{sb},\chi)=\frac{\text{constant}}{g_{sb}}. \tag{3}$$

In this case, the probability of collision between two particles (s and b) is independent of their velocities (v_s and v_b), and we consider the escape of a minor ions s through a background neutrals b (we assumed one neutral species). In the present study, we confine our attention to the Monte Carlo simulation of the Maxwell molecule interactions, *i.e.*, we are interested in computing the velocity of the test ion (minor) after Maxwell molecule collision with the neutral b

In order to simulate the effect of Maxwell molecule interactions in a plasma, we introduce a Maxwell molecule model by a Monte Carlo method for a particle simulation. The Monte Carlo method is used to approximate the solution of physical problem by using random sampling. The standard procedure of the Monte Carlo simulation is to follow the motion of the minor ion (one at a time) for a short period of time, at the end of which the change in the minor ion velocity due to Maxwell molecule interactions is determined. The test ion s is injected into the simulation region with a random initial velocity that is consistent with the assumed non-drifting Maxwellian immediately below the injection region. The minor (test) ion s is considered to move for a short interval of time Δt under the influence of the external forces. The time interval between two successive collisions is randomly generated using a properly weight random number generator [5-7]. When a collision occurred, the minor ion velocity after collision was determined by using another set of random numbers having statistical properties determined according to the chosen Maxwell molecule collision model. Now, we use Monte Carlo technique to generate the initial velocity of the minor ion s. We describe the Maxwell molecule interactions and generate the period Δt between successive collisions and scattering angle, we generate the random velocity of the background neutrals b. Finally, we obtained the minor ion velocity after collision.

Outside the simulation region, the minor (test) ions s are assumed to be in static equilibrium with some thermal velocity $(2kT_s/m_s)^{1/2}$, their velocity distribution function f_s can be written as a non-drifting Maxwellian, offset in velocity,

$$f_s(v_s)=\exp\left(-m_s v_s^2/2kT_s\right). \tag{4}$$

As mentioned earlier, $\int f_s(v)dv$ gives the number density (n) of the test ions. Integrating over the entire velocity space, the velocity distribution function is then

$$f_s(v_s)=n_s\left(\frac{m_s}{2\pi kT_s}\right)^{3/2}\exp\left(-\frac{m_s v_s^2}{2kT_s}\right). \tag{5}$$

In most of space plasma investigation, the ratio of ion-neutral collision frequency v_{in} to the ion cyclotron frequency Ω_i is very small. As $v_{in}/\Omega_i\to 0$, the test ion velocity distribution function in velocity space becomes symmetric about an axis that is parallel to the magnetic field direction [8]. Because of the cylindrical symmetry, it is convenient to introduce a cylindrical coordinate system with its axis along the magnetic field. In this coordinate, the ion velocity components in the parallel and perpendicular directions of the magnetic field are denoted by $v_\parallel$ and $v_\perp$.

In the cylindrical coordinate system and in terms of $v_\parallel$ and $v_\perp$, the test velocity distribution function $f_s(v_s)$ eq (5) becomes

$$f_s(v_s)=n_s f_s(v_{\perp s})f_s(v_{\parallel s}),$$

where

$$f_s(v_{\parallel s})=\left(\frac{m_s}{2\pi kT_s}\right)^{1/2}\exp\left(\frac{-m_s v_{\parallel s}^2}{2kT_s}\right) \tag{6a}$$

$$f_s(v_{\perp s})=\left(\frac{m_s}{2\pi kT_s}\right)\exp\left(\frac{-m_s v_{\perp s}^2}{2kT_s}\right) \tag{6b}$$

$f_s(v_{\parallel s})$ and $f_s(v_{\perp s})$ represent the normalized velocity distributions of the minor (test) ions in the parallel and perpendicular directions of the magnetic field, respectively

Now, we will use random numbers generator to obtain a set of test particles distributed according to some given distributions (6a) and (6b). We need this to create the test particles and to inject them into the simulation region.

Generation of $v_{\perp s}$:

For test ions distributed according to $f_s(v_{\perp s})=\left(\frac{m_s}{2\pi kT_s}\right)\exp\left(\frac{-m_s v_{\perp s}^2}{2kT_s}\right)$, the probability of the test ion of being in some range of values $dv_{\perp s}$ is then $P(v_{\perp s})dv_\perp=2\pi v_{\perp s}f_s(v_{\perp s})$ which leads to [9]

$$P(v_{\perp s})=2v_{\perp s}\left(\frac{m_s}{2kT_s}\right)\exp\left(\frac{-m_s v_{\perp s}^2}{2kT_s}\right) \tag{7}$$

the values of $v_{\perp s}$ are given by

$$\int P(v'_{\perp s})\,dv'_{\perp s} = \text{rand}\,(\,), \tag{8}$$

where rand ( ) is a pseudo-random number with uniform probability between the limits 0.0 and 1.0, that is, taking each value of rand() in turn, we must solve eq. (8) and find the corresponding value of $v_{\perp s}$, which is shown to be

$$v_{\perp s}^2 = -\left(\frac{2kT_s}{m_s}\right)\log\left[\text{rand}\,(\,)-1\right]. \tag{9}$$

This $v_{\perp s}$ is the perpendicular velocity of the randomly injected test ion into the simulation region.

Generation of $v_{\parallel s}$:

We must notice that we are interested in test ions that are crossing the bottom boundary of the simulation region (*i.e.* $v_{\parallel s} > 0$). The probability of finding a particle with parallel velocity $v_{\parallel s}$ swept across the boundary is proportional to the flux of such particles $f_s(v_{\parallel s})v_{\parallel s}$, *i.e.* $P(v_{\parallel s}) = cv_{\parallel s}f_s(v_{\parallel s})$, where c is the normalization constant obtained from $\int_0^\infty P(v_{\parallel s})dv_{\parallel s} = 1$.

Knowing c, we get

$$P(v_{\parallel s}) = 2\left(\frac{m_s}{2kT_s}\right)v_{\parallel s}\exp\left(\frac{-m_s v_{\parallel s}^2}{2kT_s}\right) \tag{10}$$

Similar to eq. (9), the value of the test ion parallel velocity is given by

$$v_{\parallel s}^2 = -\left(\frac{2kT_s}{m_s}\right)\log\left[\mathit{rand}\,(\,)-1\right]. \tag{11}$$

The numerical values of $v_{\perp s}$ and $v_{\parallel s}$ are different from each other because of rand ( ). At this stage, we have created, at the boundary level of the simulation region, a test ion from the corresponding test velocity distribution.

The background neutrals are assumed to be in static equilibrium and, consequently, their distribution function f_b is assumed to have a Maxwellian distribution

$$f_b(v) = n_b\left(\frac{m_b}{2\pi kT_b}\right)^{3/2}\exp\left(-\frac{m_b v_b^2}{2kT_b}\right) \tag{12}$$

thus $f_b(v)$ can be written in terms of $v_{\parallel b}$ and $v_{\perp b}$

$$f_b(v) = n_b f_b(v_{\parallel b})\,f_b(v_{\perp b}) \tag{12a}$$

with

$$f_b(v_{\parallel b}) = \left(\frac{m_b}{2\pi kT_b}\right)^{3/2}\exp\left(\frac{-m_b v_{\parallel b}^2}{2kT_b}\right) \tag{12b}$$

$$f_b(v_{\perp b}) = \left(\frac{m_b}{2\pi kT_b}\right)\exp\left(\frac{-m_b v_{\perp b}^2}{2kT_b}\right) \tag{12c}$$

The generation of $v_{\perp b}$ is similar to generation of $v_{\perp s}$, therefore

$$v_{\perp b}^2 = -\left(\frac{2kT_b}{m_b}\right)\log\left[\text{rand}\,()-1\right]. \tag{13}$$

However, the generation of $v_{\parallel b}$ is different from the generation of $v_{\parallel s}$. In the case of $v_{\parallel s}$, we were interested in those test particles that can reach the boundary of the simulation region, while in $v_{\parallel b}$ case, the background neutrals exist in the simulation region.

The probability of picking up a neutral from the neutral particles of the background that are distributed according to $f_b(v_{\parallel b})$ along the direction of the magnetic field, is proportional to $f_b(v_{\parallel b})$, *i.e.*, $P(v_{\parallel b}) = cf_b(v_{\parallel b})$, where c is the proportionality constant. The integral of the probability over the whole intervals $(-\infty,\infty)$ is equal to 1:

$$\int_{-\infty}^{\infty} P(v_{\parallel b})dv_{\parallel b} = 1, \quad \text{this leads to}$$

$$P_{\parallel}(v_{\parallel b}) = \left(\frac{m_b}{2\pi\, kT_b}\right)^{1/2}\exp\left(\frac{-m_b v_{\parallel b}^2}{2kT_b}\right) \tag{14}$$

Generation of a neutral particle from the above probability distribution, is given by the following equation

$$\text{rand}() = \int_{-\infty}^{v_{\parallel b}} P(v'_{\parallel b})\,dv'_{\parallel b}. \tag{15}$$

The integral is computed

$$\text{rand}() = \frac{1}{2}\left[1+\text{erf}\left(\frac{m_b}{2kT_b}\right)\right]$$

where erf is the error function.

Hence, we obtain an explicit formula for $v_{\parallel b}$

$$v_{\parallel b} = \left(\frac{2kT_b}{m_b}\right)^{1/2}\text{erf}^{-1}\left(2\,\text{rand}()-1\right). \tag{16}$$

Eqs. (9), (11), (13) and (16) give the velocities of the colliding particles (test ion s and background neutral b). Now, we will investigate the effect of Maxwell molecule interactions on the above velocities and consequently, the velocities of the colliding particles after collision.

Our aim is to simulate the interaction of a test ion moving under the influence of an external forces through a background of neutrals atoms, these neutrals are distributed according to Maxwell distribution function with background temperature T_b. The simulation steps must provide us the time between each pair of collisions (interactions) and the change in the test ion velocity due to each collision. For a Maxwell molecule interaction, the collision frequency w is dependent of the relative velocity $\mathbf{g}_{sb} = \mathbf{v}_s - \mathbf{v}_b$.

Consider the test particle with velocity $\mathbf{v}_s$, the probability that this test particle survives at time t without suffering a collision is $P(t)$, while the quantity wdt is the probability that the test particle collide with the background neutrals between time t and $t + dt$.

The probability that a particle will suffer no collision in the interval dt is given by $P(t+dt) = P(t)(1-wdt)$, using Taylor expansion and the condition $P(0) = 1$, the probability $P(t)$ will be

$$P(t) = \exp(-wt). \tag{17}$$

In order to determine the time interval τ between collisions, we set up the equation :

$$\mathrm{rand}() = \int^{\tau} e^{-wt} dt.$$

Computing the integral on the right, we get the relation $\mathrm{rand}() = 1/w\left(1-e^{-w\tau}\right)$, and hence

$$\tau = -\log(1-(w)\,\mathrm{rand}())/w. \tag{18}$$

The mean distance travelled by the test particle between collisions is called mean free path λ and given by

$$\lambda = v_s\tau = \left(v_{\|s}^2 + v_{\perp s}^2\right)^{1/2}\left\{\frac{-1}{w}\log\left[1-w\,\mathrm{rand}()\right]\right\}, \tag{19}$$

w is the collision frequency for Maxwell molecule interaction and given by Schunk [1].

Thus, we can generate pair of particles (test and background neutral) at random. Next we calculate the changes in the velocities due to binary collisions in the time interval τ . As a result of a binary collision, the magnitude of the relative velocity $\mathbf{g}_{sb}$ is unchanged but its direction is altered by the scattering angle χ However, the velocity of the center of gravity $\mathbf{v}_{CG}$ given by

$$\mathbf{v}_{CG} = \frac{m_s\mathbf{v}_s + m_b\mathbf{v}_b}{m_s + m_b}$$

remains the same both in magnitude and direction before and after the collision.

The relative velocity and the velocity of the center of gravity after the collision are given by

$$\mathbf{g}'_{sb} = \mathbf{v}'_s - \mathbf{v}'_b \tag{20a}$$

and

$$\mathbf{v}'_{CG} = \frac{m_s\mathbf{v}'_s + m_b\mathbf{v}'_b}{m_s + m_b} \tag{20b}$$

where prime denotes after collision.

From eqs. (20a) and (20b), the velocity of test particle after collision is

$$\frac{m_b\mathbf{g}'_{sb}}{m_s + m_b} \tag{20c}$$

and similarly

$$\frac{m_b\mathbf{g}_{sb}}{m_s + m_b} \tag{20d}$$

The parallel and perpendicular components of the relative velocity $\mathbf{g}_{sb}$ are

$$g_{sb\|} = v_{s\|} - v_{b\|},$$

$$g_{sb\perp} = \left(v_{s\perp}^2 + v_{b\perp}^2 - 2v_{s\perp}v_{b\perp}\cos\varphi\right)^{1/2}, \tag{21}$$

where φ is the angle between $\mathbf{v}_{s\perp}$ and $\mathbf{v}_{b\perp}$ in the perpendicular plane.

Similarly, the parallel and perpendicular components of v_{CG} are

$$v_{CG\|} = \frac{m_s}{m_s + m_b}v_{\|s} + \frac{m_b}{m_s + m_b}v_{\|b},$$

$$v_{CG\perp} \quad \frac{m_s}{m_s + m_b}v_{\perp s} \quad \frac{m_b}{m_s + m_b}v_{\perp b}$$

$$\left.\frac{2m_sm_b}{(m_s + m_b)^2}v_{\perp s}v_{\perp b}\cos\varphi\right)^{1/2} \tag{22}$$

After collision, we are interested to determine the velocity of the test particle $\mathbf{v}'_{sb}$; however, the velocity of the background is generated randomly for each collision as shown earlier.

From eq. (20c), we have

$$v'_{\parallel s} = v_{CG\parallel} + \frac{m_b g'_{sb\parallel}}{m_s + m_b}$$

$$v_{CG\perp} \qquad \frac{m_b}{m_s + m_b} g'_{sb\perp} \qquad + \frac{2m_b}{m_s + m_b} v_{CG\perp} g'_{sb\perp} \cos\varphi' \Big)^{1/2} \tag{23}$$

where φ' is the angle between $v_{CG\perp}$ and $g'_{sb\perp}$ in the perpendicular plane, $g'_{sb\parallel} = g\cos\theta'$, θ' is the angle between the relative velocity g' and the parallel direction and $g'_{sb\perp} = \left(g^2 - g'^2_{sb\parallel}\right)^{1/2}$.

Now, the question arises as to how to select the random directions, *i. e.* the angles φ, φ' and θ'. The angles φ and φ' take on values from 0 to 2π and are chosen randomly with a uniform distribution between 0 and 2π.

The formulas for construction of φ and φ' will be written

$$\varphi = 2\pi \text{ rand( )}$$

and

$$\varphi' = 2\pi \text{ rand( )}. \tag{24}$$

However, the cosine of the angle $\theta'(\cos\theta')$, be uniformly distributed over the interval $[-1, 1]$. The formula for constructing $\cos\theta'$ follows:

$$\cos\theta' = 2 \text{ rand( )} - 1. \tag{25}$$

The values of rand() in these formulas should of course, be different

We have presented a Monte Carlo method for a Maxwell molecule interaction. The major steps of the Monte Carlo simulation are

(i) Test ion (minor) is randomly generated (*i.e.* $v_{\parallel s}$ and $v_{\perp s}$ are determined) from a non-drifting Maxwellian distribution (of temperature T_s)

(ii) The time interval between collisions is randomly generated such that it has an exponential probability density function (*i.e.* $P(t) = e^{-wt}$)

(iii) The final velocity of the test ion due to the external forces is computed.

(iv) A neutral particle from the background is randomly chosen from a Maxwellian distribution (of temperature T_b).

(v) The relative velocity $\boldsymbol{g}$ and the velocity of the center of gravity $\boldsymbol{v}_{CG}$ between the colliding particles (test ion s and neutrals b) are computed. While $\boldsymbol{v}_{CG}$ is the same before and after collision both in magnitude and direction, the magnitude of $\boldsymbol{g}$ remaining same, its direction after collision is changed.

(vi) $\boldsymbol{v}_{CG}$ and $\boldsymbol{g}$ after collision are used to calculate the velocity of the test ion $(\boldsymbol{v}'_s)$ after collision.

Steps 2-6 are repeated using this velocity $(\boldsymbol{v}'_s)$ as the initial test ion velocity.

The result of such procedure gives information about the test ion (minor) for a long period of time.

Time average of various kinds can be computed from such data; this time, averages have been set equal to the instantaneous averages over the assembly, in accordance with the Ergodic theory.

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