Monte Carlo simulations of a diffusive shock with multiple scattering angular distributions

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Abstract: We independently develop a simulation code to research the previous dynamical Monte Carlo simulation of a diffusive shock under the isotropic scattering law during the scattering process, and the same results are obtained. We extend the prescribed scattering law to include an anisotropic scattering law for further developing this dynamical Monte Carlo simulation. We find that the prescribed scattering law has an important effect on the final energy spectrum.

Keywords: acceleration of particles– shock wave– method– numerical

1 Introduction

It is well known that the diffusive acceleration model has been popular for more than five decades since Fermi [7] first proposed that cosmic rays could be produced via diffusive processes. Until now, diffusive shock acceleration (DSA) has been extensively applied to many physical systems, such as shocks in the solar system, in our Galaxy, and throughout the Universe [1, 2, 3]. The nonlinear interactions in plasma usually include such things as the turbulence of scattering wave field, cosmic ray (CR) injection, and “back reaction” by CR pressure. These complex behaviors have held back comprehensive understanding of the DSA and nonlinear DSA theory. Therefore, to study the properties of the acceleration process and dynamical behavior of the CR’s “back reaction” on the background flow, choosing numerical simulation methods has been a primary and essential problem [11, 10, 6, 12, 5]. There are four main simulation methods: Monte Carlo method, hybrid simulation, two-fluid model, and kinetic simulation[8].

In an effort to follow and extend the previous dynamical Monte Carlo simulation [9], we independently developed a simulation code based on the Matlab platform using multiple scattering laws. In Section 2, the simulation model and PIC techniques are described. In Section 3, the simulation results are presented. Section 4 includes the conclusions.

2 The model

The dynamical Monte Carlo simulation has been developed by Knerr et al. [9] to study Earth’s bow shocks. It gives good results for the higher than 1MeV cutoff in energy particles and the power-law energy tail in the energy spectra. To validate these consistent results from the previous model and extend this study to find what might be responsible for the shock compression ratio, we extend the previous isotropic scattering angular law by including an anisotropic scattering angular law. This prescribed multiple scattering law consists of an isotropic and an anisotropic scattering angular distribution. The scattering angular variables arise from the pitch angle and the azimuthal angle, and they are described by the Gaussian function \( f(\delta \theta, \delta \phi) \). Once a particle has a collision with the massive scattering centers, its pitch angle becomes \( \theta' = \theta + \delta \theta \), and the azimuthal angle becomes \( \phi' = \phi + \delta \phi \), where \( \delta \theta \) is the variation in the pitch angle \( \theta \), and \( \delta \phi \) is the variation in the azimuthal angle \( \phi \). The \( \sigma \) and \( \mu \) are used to represent the standard deviation value and the average value of Gaussian function \( f(\delta \theta, \delta \phi) \), respectively. We catalog the four cases as follows. (1) Case A: \( \sigma = \pi/4, \mu = 0 \). (2) Case B: \( \sigma = \pi/2, \mu = 0 \). (3) Case C: \( \sigma = \pi, \mu = 0 \). (4) Case D: \( \sigma = \infty, \mu = 0 \).

As shown in Figure 1, one particle’s box frame velocity \( V \) is a total velocity, which is composed of the local thermal velocity \( V_L \) and the bulk fluid speed \( U \) (i.e. \( V = V_L + U \)), for upstream \( U = U_0 \), for downstream \( U = 0 \). After one particle arrives in the downstream region, its kinetic energy is converted into random thermal energy by dissipation processes. With the development of these many processes, the bulk fluid speed of downstream flow becomes zero, and the length of downstream region is extended dynamically.

As listed in Table 1[9], all of the specific parameters are used in our simulations, considering PIC techniques. In summary, these new codes consist of the following three substeps like the previous simulation, except for the third substep employing the extended multiple scattering laws.
Figure 1: The simulation box [9].

Table 1: The parameters of the simulated cases

| Inflow velocity | \( u_0 = 0.2 \) | 40.3 km/s |
|-----------------|----------------|----------|
| Thermal speed   | \( v_{th} = 0.2 \) | 26.9 km/s |
| Scattering time | \( \tau = 0.13 \) | s        |
| Box size        | \( x_{max} = 300 \) | \( 10R_e \) |
| Total time      | \( t_{max} = 2400 \) | 6 minutes |
| Time step size  | \( dt = 1/130 \) | 0.00535 s |
| Number of zones | \( n_z = 600 \) |          |
| Initial particles per cell | \( n_0 = 500 \) |          |
| FEB distance    | \( X_{feb} = 90 \) | \( 3H_e \) |

**Notes:** \( R_e \) is the Earth’s radius, the Mach number \( M = 11.6 \). Dimensionless numbers are used in the simulations [9].

(i) Individual particles move. Particles with their velocities move along the one-dimensional \( x \) axis:

\[
X_k^t = X_k^{t-1} + (V_x)_k \tau, t \in [1, t_{max}], k \in [1, k_{max}], \quad (1)
\]

\[
(V_x)_k = (V_{Lx})_k + (U_x)_k, \quad (2)
\]

\[
(U_x)_k = \frac{1}{n_k} \sum_{i=1}^{n_k} (V_x)_i, \quad (3)
\]

where \( t_{max} = 72000 \), \( k_{max} = 600 \), and “\( k \)” is the index of the grid, \( (U_x)_k \) represents the bulk fluid speed of the computational grid along to the \( x \) direction, and the value of \( U_k \) is obtained from substep (ii). (ii) Mass collection. Summation of particle masses and velocities are calculated at the center of each computational grid:

\[
P_k = \sum_{i=1}^{n_k} m_p (V_x)_i, k = 1, 2, \ldots k_{max} \quad (4)
\]

\[
U_k = \frac{1}{n_k} \sum_{i=1}^{n_k} (V)_i, k = 1, 2, \ldots k_{max} \quad (5)
\]

where \( n_k \) is the number density of particles in the “\( k \)” grid, representing the mass of the computational grid. Here, \( P_k \) is the total momentum of the “\( k \)” grid, \( m_p \) is the mass of proton, and \( U_k \) is the average bulk fluid speed of the grid. The collected grid-based mass and momentum densities will directly decide the velocity of the scattering center \( U_k \).

The particle’s total velocity \( V \) in the box frame is decided by Equation (2). (iii) Applying multiple scattering laws. A certain fraction of the particles are chosen to scatter the background scattering center with their corresponding scattering angles according to the prescribed scattering angular distributions. The average number of scattering events occurring in an increment of time \( dt \) depends on the scattering time scale \( \tau \), and the scattering rate is presented by \( R_s = dt/\tau \), where \( R_s \) is the probability of the scattering events occurring in an increment of time. The candidates with their local velocities and scattering angles scatter off the grid-based scattering centers. These individual particles do not change their routes until they are selected to scatter once again. So the particle’s mean free path is proportional to the local thermal velocities in the local frame. For simplicity, we take its formula as \( \lambda = V_{th} \cdot \tau \). For the individual protons, the grid-based scattering center can be seen as a sum of individual momenta. So these scattering processes can be taken as the elastic collisions. One complete time step consists of the above three substeps. The total simulation evolves by repeating this time step sequence. The presented each case can occupy the CPU time for about seven weeks on a 3.4GHZ (MF) CPU per core.

### 3 Results & discussions

We present all of the shock profiles for the shock simulations of the four cases in Figure 2, and we present all aspects of simulation results including the shock structures, compression ratios, and energy spectrum, as well as the correlations between the shock compressions with the energy spectral index. For the convenience of comparison and discussion, we list the specific calculated items in Table 2. The last two rows are shown as scaled values.

![Table 2: The calculated results](image-url)

As shown in Figure 2, the present isotropic Case D largely appears similar to the results from previous dynamical simulations by Knerr et al. [9]. In addition, all aspects of the shock wave structure, density and velocity profiles, com-
3.1 Shock Profiles

Figure 2 shows time sequences of the density profiles of four cases. In each plot, a shock forms and moves away from the reflective wall. We can see that both the shock position and the FEB position are moving with a virtually constant velocity from the begin to the end of the simulation in each case. Simultaneously, as far as the positions of the FEB are concerned, we can see that the FEB position at the end of the simulation is significantly different in four different cases. As for the average density fluctuation in the downstream region, there are also apparent changes in different cases, case A has the slowest shock propagation speed among these four cases, and Case D has the lowest average density profile in the downstream region. Because from Cases A to D the only difference is the prescribed scattering angular distribution, we consider that a difference of approximately 40.93% of the shock velocity is contributed by the scattering angle distribution.

3.2 Compression ratios

Here, we compare the compression ratios calculated from the velocity profiles with those from the density profiles. First, the value of the total compression ratio can simply be calculated from the formula $r_n = u_1/u_2$, where $u_1 = u_0 + |v_{sh}|$, $u_2 = |v_{sh}|$, and $u_1$ ($u_2$) is the upstream (downstream) velocity in the shock frame. The shock velocity at the end of the simulation can be derived from the formula $v_{sh} = (X_{max} - X_{sh})/T_{max}$, where the values of $X_{max}$, $T_{max}$, and $X_{sh}$ can be seen in Table 2.

But in terms of the specific shock structure as seen in Figure 3, an accurate subshock compression ratio calculation should be more complicated. In any one of the cases in Figure 3 (plotted in the box reference frame), we show the specific aspects of a shock modified by an energetic particle population whose mean-free-path is an increasing function of momentum. The shock structure in each plot consists of three main parts: precursor, subshock, and downstream. The smooth precursor is on the largest length scale between the FEB and near shock position $X_{sh}$, where the fluid speed gradually decreases from value $U_0$ to $v_{sub}$. The size of this precursor is almost the mean-free-path length of the maximum energy accelerated particles. The smallest scales is the subshock region with a sharp deflection of the fluid speed decreasing from $v_{sub}$ to $v_{box}$. The downstream region changes after the fluid speed becomes $v_{box} = 0$ by microphysical dissipation processes. The gas subshock is just an ordinary discontinuous classical shock embedded in the comparably larger scale energetic particle shock [4]. The value of $v_{sub}$ is determined by a sharp deflection of smooth curves in velocity profiles near the shock front, and the value of the subshock velocity increases from cases A, B, and C to Case D (i.e. $(v_{sub})_A < (v_{sub})_B < (v_{sub})_C < (v_{sub})_D$). All of the velocity profiles are based on the box frame. That value of the box frame’s velocity $v_{box}$ is zero in all cases. The subshock compression ratio $r_{sub}$ is calculated from the formula $r_{sub} = (v_{sub} + |v_{sh}|)/v_{sh}$. The values of $r_{sub}$ are shown in Table 2 on the same shock frame reference.

We then calculate the total compression ratios from the density profiles in Figure 4. $r_p = \rho_2/\rho_1$, where $\rho_1$ ($\rho_2$) is the upstream (downstream) density, and $\rho_2$ is decided by

$$\rho_2 = \frac{1}{(k_{max} - k_{sh})} \sum_{k=k_{sh}}^{k_{max}} n_k$$

where $n_k$ is the number density of particles in the “k” grid, $k_{sh} = x_{sh}/dx$ is the index of the shock position at the end of the simulation, and $k_{max}$ is the grid index of the $X_{max}$. As shown in Figure 4, the upstream density $\rho_1$ is the same constant value $n_0$ in each case. The downstream density $\rho_2$ decreases from cases A, B, and C to Case D (i.e. $(\rho_2)_A > (\rho_2)_B > (\rho_2)_C > (\rho_2)_D$). As listed in Table 2, the values of the subshock compression ratios $(r_{sub})_A=2.5421$, $(r_{sub})_B=2.5421$, $(r_{sub})_C=2.5421$, and $(r_{sub})_D=2.5421$. The values of $\rho_2$ are significant in all cases.
Spectra calculated in the shock frame from the initial and final particle (proton) energy distributions in all cases are shown in Figure 5. The energy units in this plot are derived from the scaling parameters presented in Table 1. Initially, all particles move toward the wall with a certain thermal spread in energy. A narrow peak at $E=1.3105\text{keV}$ represents the initial Maxwell energy distribution. The four extended curves indicate the final energy spectral distribution, averaged over the entire downstream region, corresponding to the four cases, respectively. The majority of the particles cross the shock only once, producing an expanded energy spectrum with a central peak at $E_A \sim 0.05\text{keV}$, $E_B \sim 0.1\text{keV}$, $E_C \sim 0.15\text{keV}$, and $E_D \sim 0.2\text{keV}$ in Cases A, B, C, and D, respectively. However, as is shown in Figure 5, the minority of the particles gain enough energy via the Fermi acceleration mechanism to produce the “power-law” tail in the energy spectrum with the cutoff at $E_A=1.10\text{MeV}$, $E_B=2.41\text{MeV}$, $E_C=2.98\text{MeV}$ and $E_D=4.01\text{MeV}$ corresponding to Cases A, B, C and D, respectively. The shock energy spectral indices are shown in Table 2.

**4 Conclusions**

In conclusion, by the comparison of the calculated results from different extended cases, we find that the total energy spectral index increases as the standard deviation value of the scattering angular distribution increases, but the subshock's energy spectral index decreases as the standard deviation value of the scattering angular distribution increases. Specifically, the cases of applying an anisotropic scattering angular distribution will produce a slightly harder subshock's energy spectrum, and the case of applying an isotropic scattering angular distribution will produce a slightly softer subshock's energy spectrum.

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