

A Complementary Fluid Method in δf Particle Simulation

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A new simulation method that improves the conservation properties of δf particle simulation for the collisionless Boltzmann equation is presented. When the distribution function is divided into a reference distribution specified in advance and a variation distribution, the time evolution of the variation distribution is described by an advection term in the phase space and a source term associated with the reference distribution. The time evolution of the Klimontovich distribution function of the δf method was investigated. It is shown that the errors in the Monte Carlo estimate of the source term in the δf method deteriorate the conservation properties. In the new simulation method, errors in the Monte Carlo estimate of the source term are corrected with a complementary fluid model. An example of the complementary fluid model is presented for bump-on-tail instability. The simulation results are compared with those of the conventional δf method. It is demonstrated that particle, momentum, and energy are well conserved with the new simulation method.

Keywords:

collisionless Boltzmann equation, Vlasov equation, computer simulation, δf method, fluid method, conservation properties

1. Introduction

In δf particle simulation [1-4], the distribution function is represented by the sum of a reference distribution and a variation distribution, often represented by f_0 and δf , respectively. In the δf method, Lagrangian markers (macro particles) are employed to estimate δf , but not the total distribution function $f = f_0 + \delta f$. In particle simulations of plasmas, the number of Lagrangian markers is much smaller than that of real plasma particles. Thus, we cannot eliminate the errors in the Monte Carlo estimates with Lagrangian markers. The errors in the estimate lead to “numerical noise” in particle simulations. In the δf method, as contribution from f_0 is calculated accurately, the errors in the estimate are in proportion to δf . If $|\delta f / f_0| \ll 1$, the δf method significantly reduces the numerical noise compared to the total f method.

A drawback of the δf method is that conservation properties, i.e., the conservation of particle, momentum, and energy, are not guaranteed [3,4], although a well-chosen initial distribution of Lagrangian markers improves them [5]. When the distribution is divided into f_0 and δf , the time evolution of δf is described by an advection term of δf and a linear source term associated with f_0 . In the δf method, δf is approximated by the Klimontovich distribution function δf_K using Lagrangian markers. In the time evolution of δf_K , the advection term of δf_K can be written in conservative form and does not violate the conservation properties. On the other hand, the linear source term, which is a Monte Carlo estimate in the δf method, violates the conservation properties.

We present a new simulation method where the δf scheme is complemented with fluid models to correct the errors in the estimate of the source term. The new method is different from the split-weight particle scheme [6], which is a δf method where the chosen f_0 is dependent on the electrostatic potential. In Sec. 2, we will discuss why the δf method lacks conservation properties and present the new simulation method. Sec. 3 is devoted to the demonstration of the conservation properties of the new method. The simulation results of bump-on-tail instability with the new method are presented and compared with those of the conventional δf simulation. A summary is given in Sec. 4.

2. Complementary Fluid Method in the δf Particle Simulation

Let us start by introducing the collisionless Boltzmann equation (Vlasov equation):

$$\frac{df}{dt} = \frac{\partial}{\partial t} f + \dot{\mathbf{Z}} \cdot \frac{\partial f}{\partial \mathbf{Z}} = 0, \tag{1}$$

where $Z^i (i = 1, 2, 3, \dots, M)$ are generalized coordinates in M -dimensional phase space. The distribution function $f(\mathbf{Z}, t)$ in the phase space is defined such that $f d\Gamma$ is the number of particles in the volume element $d\Gamma = \mathcal{J} dZ^1 dZ^2 \dots dZ^M$, where $\mathcal{J}(\mathbf{Z}, t)$ is the Jacobian. In this letter, we assume that the Liouville theorem holds; i.e.,

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$$\frac{\partial}{\partial t} \mathcal{J} + \frac{\partial}{\partial \mathbf{Z}} \cdot (\dot{\mathbf{Z}} \mathcal{J}) = 0. \quad (2)$$

In the δf particle simulation method, the distribution function is approximated by f_D , the sum of the reference distribution f_0 and the Klimontovich distribution function δf_K of Lagrangian markers [4]:

$$f_D(\mathbf{Z}, t) = f_0(\mathbf{Z}, t) + \delta f_K(\mathbf{Z}, t), \quad (3)$$

$$\delta f_K(\mathbf{Z}, t) = \frac{1}{\mathcal{J}(\mathbf{Z}, t)} \sum_{j=1}^N w_j(t) \delta(\mathbf{Z} - \mathbf{Z}_j(t)), \quad (4)$$

$$w_j(t) = \frac{1}{N} \frac{\delta f(\mathbf{Z}_j, t)}{p(\mathbf{Z}_j)}, \quad (5)$$

where N is the total number of Lagrangian markers. The probability density of Lagrangian markers $p(\mathbf{Z}, t)$ satisfies

$$\int_V p(\mathbf{Z}) d\Gamma = 1 \quad (6)$$

in the phase space volume V . The marker probability density is constant along each marker orbit because the Liouville theorem holds. The Monte Carlo estimate for the general moment integral is given by

$$\begin{aligned} I(A) &\equiv \int_V A(\mathbf{Z}) f_D(\mathbf{Z}) d\Gamma \\ &= \int_V A(\mathbf{Z}) [f_0(\mathbf{Z}) + \delta f_K(\mathbf{Z})] d\Gamma \\ &= \int_V A(\mathbf{Z}) f_0(\mathbf{Z}) d\Gamma + \sum_{j=1}^N w_j A(\mathbf{Z}_j). \end{aligned} \quad (7)$$

The time evolution of the particle weight w_j is obtained from the collisionless Boltzmann equation, Eq. (1),

$$\begin{aligned} \frac{dw_j}{dt} &= \frac{1}{N} \left[\frac{1}{p(\mathbf{Z}_j)} \frac{d\delta f(\mathbf{Z}, t)}{dt} \right]_{\mathbf{Z}=\mathbf{Z}_j} \\ &= -\frac{1}{N} \left[\frac{1}{p(\mathbf{Z}_j)} \frac{df_0(\mathbf{Z}, t)}{dt} \right]_{\mathbf{Z}=\mathbf{Z}_j}, \\ &= -\frac{1}{N} \left[\frac{1}{p(\mathbf{Z}_j)} \left(\frac{\partial f_0(\mathbf{Z}, t)}{\partial t} + \dot{\mathbf{Z}} \cdot \frac{\partial f_0(\mathbf{Z}, t)}{\partial \mathbf{Z}} \right) \right]_{\mathbf{Z}=\mathbf{Z}_j}. \end{aligned} \quad (8)$$

We multiply Eq. (4) by $\mathcal{J}(\mathbf{Z}, t)$ and take the time derivative. This yields

$$\frac{\partial}{\partial t} (\mathcal{J} \delta f_K) = \sum_{j=1}^N \frac{dw_j}{dt} \delta(\mathbf{Z} - \mathbf{Z}_j) - \sum_{j=1}^N w_j \left[\dot{\mathbf{Z}}_j \cdot \frac{\partial}{\partial \mathbf{Z}} \delta(\mathbf{Z} - \mathbf{Z}_j) \right]. \quad (9)$$

Using relations $\frac{\partial}{\partial \mathbf{Z}} \cdot \dot{\mathbf{Z}}_j(t) = 0$ and $\frac{\partial}{\partial \mathbf{Z}} w_j(t) = 0$, the second term of the right-hand side of Eq. (9) is rewritten to

$$\begin{aligned} & -\sum_{j=1}^N w_j \left[\dot{\mathbf{Z}}_j \cdot \frac{\partial}{\partial \mathbf{Z}} \delta(\mathbf{Z} - \mathbf{Z}_j) \right] \\ &= -\sum_{j=1}^N \frac{\partial}{\partial \mathbf{Z}} \cdot [\dot{\mathbf{Z}}_j w_j \delta(\mathbf{Z} - \mathbf{Z}_j)] \end{aligned} \quad (10)$$

$$= -\sum_{j=1}^N \frac{\partial}{\partial \mathbf{Z}} \cdot [\dot{\mathbf{Z}} w_j \delta(\mathbf{Z} - \mathbf{Z}_j)] \quad (11)$$

$$= -\frac{\partial}{\partial \mathbf{Z}} \cdot (\dot{\mathbf{Z}} \mathcal{J} \delta f_K). \quad (12)$$

Then, Eq. (9) is rewritten to

$$\frac{\partial}{\partial t} (\mathcal{J} \delta f_K) + \frac{\partial}{\partial \mathbf{Z}} \cdot (\dot{\mathbf{Z}} \mathcal{J} \delta f_K) = \sum_{j=1}^N \frac{dw_j}{dt} \delta(\mathbf{Z} - \mathbf{Z}_j). \quad (13)$$

We see that the left-hand side of Eq. (13) is written in conservative form while the right-hand side is not. Thus, without the right-hand side, the δf Klimontovich distribution function, or the δf method, would have the conservation properties. We should notice that the right-hand side is a Monte Carlo estimate of

$$\begin{aligned} & -\left[\frac{\partial}{\partial t} f_0(\mathbf{Z}, t) + \dot{\mathbf{Z}} \cdot \frac{\partial}{\partial \mathbf{Z}} f_0(\mathbf{Z}, t) \right] \mathcal{J}(\mathbf{Z}, t) \\ &= -\frac{\partial}{\partial t} [\mathcal{J}(\mathbf{Z}, t) f_0(\mathbf{Z}, t)] - \frac{\partial}{\partial \mathbf{Z}} \cdot [\mathcal{J}(\mathbf{Z}, t) f_0(\mathbf{Z}, t) \dot{\mathbf{Z}}]. \end{aligned} \quad (14)$$

Equation (14) is clearly in conservative form. The error in the Monte Carlo estimate in the right-hand side of Eq. (13) spoils the conservation properties of the δf method.

Let us consider a complementary distribution function $g(\mathbf{Z}, t)$ that evolves by

$$\begin{aligned} & \frac{\partial}{\partial t} [\mathcal{J}(\mathbf{Z}, t) g(\mathbf{Z}, t)] + \frac{\partial}{\partial \mathbf{Z}} \cdot [\dot{\mathbf{Z}} \mathcal{J}(\mathbf{Z}, t) g(\mathbf{Z}, t)] \\ &= -\left[\frac{\partial}{\partial t} f_0(\mathbf{Z}, t) + \dot{\mathbf{Z}} \cdot \frac{\partial}{\partial \mathbf{Z}} f_0(\mathbf{Z}, t) \right] \mathcal{J}(\mathbf{Z}, t) \\ & \quad - \sum_{j=1}^N \frac{dw_j}{dt} \delta(\mathbf{Z} - \mathbf{Z}_j). \end{aligned} \quad (15)$$

It is clear that the sum of the two distributions, $\delta f_C \equiv \delta f_K + g$ satisfies

$$\begin{aligned} & \frac{\partial}{\partial t} [\mathcal{J}(\mathbf{Z}, t) \delta f_C(\mathbf{Z}, t)] + \frac{\partial}{\partial \mathbf{Z}} \cdot [\dot{\mathbf{Z}} \mathcal{J}(\mathbf{Z}, t) \delta f_C(\mathbf{Z}, t)] \\ &= -\left[\frac{\partial}{\partial t} f_0(\mathbf{Z}, t) + \dot{\mathbf{Z}} \cdot \frac{\partial}{\partial \mathbf{Z}} f_0(\mathbf{Z}, t) \right] \mathcal{J}(\mathbf{Z}, t). \end{aligned} \quad (16)$$

The time evolution of $\delta f_C = \delta f_K + g$ is written in conservative form without the error in the estimate of the source term. This indicates that the complementary distribution g will improve the conservation properties and the accuracy of the δf method.

It is not an easy task to calculate Eq. (15). However,

in many applications, it is not necessary to keep detailed information of the distribution function. What are needed are the low-order moments, such as number density, momentum density, and pressure. In this letter, we propose following the time evolution of the low-order moments of g using fluid equations. We should notice that the fluid models are applied only to correct the errors in the estimate of the source term.

The complementary fluid equations must be derived from Eq. (15). It is well known that the collisionless Boltzmann equation does not give the equation for the highest-order moment. Additional physics or an additional assumption is needed for the closure of the fluid equations. It is beyond the scope of this letter to discuss the best closure model and the best numerical method for the fluid equations, which may depend on the problem to be solved. In the next section, we will present an example of the complementary fluid model for bump-on-tail instability.

3. Application to Bump-on-Tail Instability

The new simulation method was applied to the bump-on-tail instability of electrons. Bump-on-tail instability is an inverse Landau damping due to the reversed gradient in the velocity space. Here, we consider a 1-dimensional phase space (x, v) . Ions are assumed to be immobile and to have a constant number density n_0 . The initial distribution of electrons is

$$f(x, v, t=0) = (n_0 - n_f) \frac{1}{\sqrt{2\pi}v_t} e^{-v^2/2v_t^2} + n_f \frac{1}{\sqrt{2\pi}v_t} e^{-(v-v_0)^2/2v_t^2}, \quad (17)$$

where n_f is the number density of the bump and v_t is the thermal velocity. The central velocity of the bump is v_0 . The distribution function evolves following the Vlasov equation:

$$\frac{\partial}{\partial t} f(x, v, t) + v \frac{\partial}{\partial x} f(x, v, t) + \frac{(-e)E}{m} \frac{\partial}{\partial v} f(x, v, t) = 0, \quad (18)$$

where $-e$, m , and E are electron charge, electron mass, and electric field in the x direction, respectively. The electric field satisfies the Maxwell equation:

$$\frac{\partial E(x, t)}{\partial x} = \frac{(-e)n(x, t) + en_0}{\epsilon_0}, \quad (19)$$

$$n(x, t) = \int_{-\infty}^{\infty} f(x, v, t) dv. \quad (20)$$

Here, ϵ_0 is the vacuum electric permittivity.

The central velocity of the bump is chosen as $v_0 = 5 v_t$. The density of the bump is $n_f/n_0 = 10^{-2}$. At $v = 4 v_t$, the initial distribution $f(x, v, t=0)$ has a reversed gradient in the velocity space. Thus, a Langmuir wave with the wave number $k = \omega_{pe}/4v_t$ is unstable. For investigation of this wave number, the length of the periodic simulation domain is $L = 8\pi v_t/\omega_{pe}$, where $\omega_{pe} = \sqrt{n_0 e^2 / \epsilon_0 m}$ is the plasma frequency.

Two simulation runs were carried out with the conventional δf method and the new method, respectively. In both runs, the Lagrangian markers were loaded uniformly in the phase space, $0 \leq x \leq L$, $-4v_t \leq v \leq 8v_t$. The initial velocity was scrambled with the bit-reversed technique [7]. The probability density of Lagrangian markers is uniform $p(x, v) = 1/V$, where V is the phase space volume and $V = 12v_t L$. The position and velocity of Lagrangian markers evolve according to the Newton equation,

$$\dot{x}_j = v_j, \quad (21)$$

$$\dot{v}_j = \frac{(-e)}{m} E(x_j, t), \quad (22)$$

where j is the index of Lagrangian markers. The reference distribution f_0 is chosen such that $f_0(v) = f(x, v, t=0)$. The weight of the markers evolves according to Eq. (8),

$$\begin{aligned} \frac{dw_j}{dt} = & -\frac{V}{N} \frac{(-e)}{m} E(x_j, t) \\ & \times \left[(n_0 - n_f) \frac{1}{\sqrt{2\pi}v_t} \left(\frac{-v_j}{v_t^2} \right) e^{-v_j^2/2v_t^2} \right. \\ & \left. + n_f \frac{1}{\sqrt{2\pi}v_t} \frac{v_0 - v_j}{v_t^2} e^{-(v_j - v_0)^2/2v_t^2} \right], \quad (23) \end{aligned}$$

$$w_j(t=0) = 0. \quad (24)$$

In the conventional δf simulation, the electron number density is estimated using the δf Klimontovich distribution function:

$$n(x, t) = n_0 + \delta n_K(x, t), \quad (25)$$

$$\delta n_K(x, t) \equiv \sum_{j=1}^N w_j S(x - x_j), \quad (26)$$

where $S(x - x_j)$ is a shape factor. For the present electrostatic problem, the system is closed with the number density, the lowest velocity moment. For the investigation of conservation properties, we calculated the time evolutions of the momentum density $M(x, t)$ and pressure $P(x, t)$ of the electrons.

$$M(x, t) = M_0 + \delta M_K(x, t), \quad (27)$$

$$M_0 = \int_{-\infty}^{\infty} m v f_0(v) dv, \quad (28)$$

$$\delta M_K(x, t) = \sum_{j=1}^N w_j m v_j S(x - x_j), \quad (29)$$

$$P(x, t) = P_0 + \delta P_K(x, t), \quad (30)$$

$$P_0 = \int_{-\infty}^{\infty} m v^2 f_0(v) dv, \quad (31)$$

$$\delta P_K(x, t) = \sum_{j=1}^N w_j m v_j^2 S(x - x_j). \quad (32)$$

We should notice that n_0 , M_0 , and P_0 are constant in space and time.

In the simulation complemented with the fluid model, the equations for the number density and the momentum density are derived from Eq. (15) while the isothermal model is assumed for the equation for pressure evolution. The following fluid equations are employed in the complemented simulation:

$$\frac{\partial}{\partial t} \delta n_g(x, t) = -\frac{1}{m} \frac{\partial}{\partial x} \delta M_g(x, t) - \sum_{j=1}^N \frac{dw_j}{dt} S(x - x_j), \quad (33)$$

$$\begin{aligned} \frac{\partial}{\partial t} \delta M_g(x, t) = & -\frac{\partial}{\partial x} \delta P_g(x, t) \\ & + (-e)E(x, t)[n_0 + \delta n_g(x, t)] \\ & - \sum_{j=1}^N \frac{dw_j}{dt} m v_j S(x - x_j), \end{aligned} \quad (34)$$

$$\begin{aligned} \frac{\partial}{\partial t} \delta P_g(x, t) = & -v_t^2 \frac{\partial}{\partial x} \delta M_g(x, t) \\ & + \frac{2(-e)}{m} E(x, t)[M_0 + \delta M_g(x, t)] \\ & - \sum_{j=1}^N \frac{dw_j}{dt} m v_j^2 S(x - x_j), \end{aligned} \quad (35)$$

$$\delta n_g(x, t=0) = 0, \quad (36)$$

$$\delta M_g(x, t=0) = 0, \quad (37)$$

$$\delta P_g(x, t=0) = 0. \quad (38)$$

The spatial derivatives are calculated with the spectrum method. In the complemented simulation, the number density, momentum density, and pressure are given by

$$n(x, t) = n_0 + \delta n_K(x, t) + \delta n_g(x, t), \quad (39)$$

$$M(x, t) = M_0 + \delta M_K(x, t) + \delta M_g(x, t), \quad (40)$$

$$P(x, t) = P_0 + \delta P_K(x, t) + \delta P_g(x, t). \quad (41)$$

In both the conventional δf and the complemented simu-

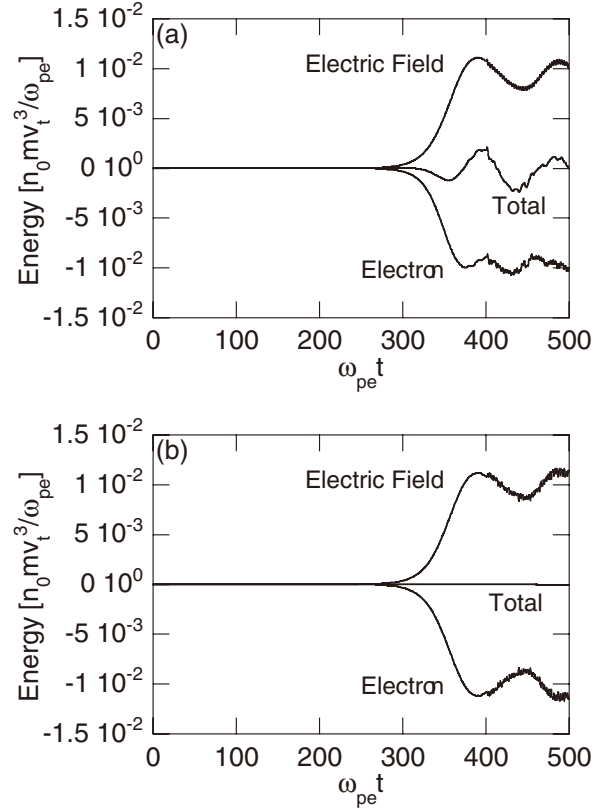


Fig. 1 Time evolution of the variations of electron kinetic energy, electric field energy and total energy in the simulation results (a) with the conventional δf method and (b) with the complementary fluid method.

lation runs, the number of grid points is 128, the time step width $\Delta t = 0.2 \omega_{pe}^{-1}$, and the number of Lagrangian makers $N = 32768$. The 4th-order Runge-Kutta method is employed for the time integration. A random and small perturbation is given to the initial particle weight. Bump-on-tail instability takes place and is saturated by particle trapping. The time evolutions of the variations of electron kinetic energy, electric field energy and total energy with the conventional δf method and with the complemented method are compared in Fig. 1. The variation of electron kinetic energy plotted in Fig. 1 is defined by $\int_0^L \frac{1}{2} (P(x, t) - P_0) dx$, where $P(x, t)$ is calculated by Eq. (30) or Eq. (41), respectively.

We see good conservation properties in the complemented simulation results. The absolute value of the total energy variation is less than 8×10^{-5} in the units of Fig. 1 for the complemented simulation. The time evolutions of the variations in total number of particles and momentum are compared in Figs. 2 and 3, respectively. The variations in total number of particles and momentum are defined by $\int_0^L (n(x, t) - n_0) dx$ and $\int_0^L (M(x, t) - M_0) dx$. We see an excellent conservation of particles for the complemented simulation, where the absolute value of the variation is 10^{-13} in the units of Fig. 2. Momentum is also well conserved for the complemented simulation, where the absolute value of the variation is 3×10^{-6} in the units of Fig. 3.

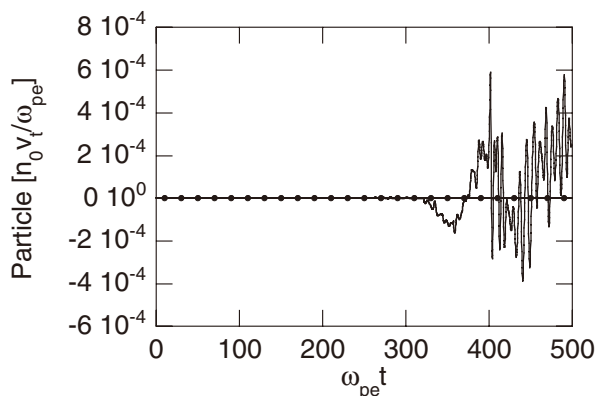


Fig. 2 Time evolution of the variations of total number of particles. The line with closed circles represents the simulation results with the complementary fluid method while the solid curve represents those with the conventional δf method.

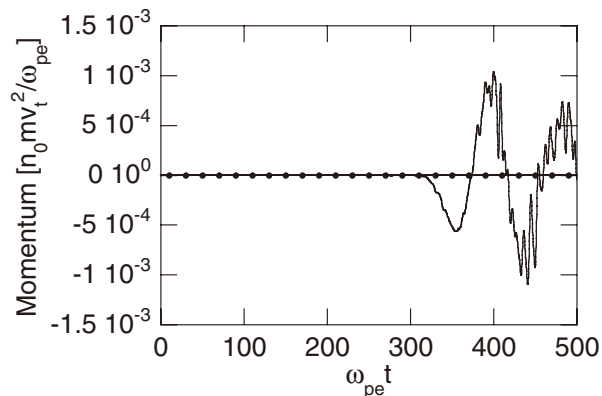


Fig. 3 Time evolution of the variations of momentum. The line with closed circles represents the simulation results with the complementary fluid method while the solid curve represents those with the conventional δf method.

4. Summary

We have presented a new simulation method for the collisionless Boltzmann equation. In the new simulation method, the δf particle method is complemented by the fluid model to correct the errors in the Monte Carlo estimate of the source term. The fluid model improves the conservation of particle, momentum, and energy. The new method was applied to bump-on-tail instability, and the results were compared with those of the conventional δf method. We demonstrated that particle, momentum, and energy are well conserved with the new simulation method.

Collisional systems and systems with source and sink require the δf method for such systems, since the complementary fluid models are employed only to correct errors in the Monte Carlo estimate. The complementary fluid models must be consistent with the Boltzmann equation of such systems. We would like to emphasize that the new simulation method presented in this letter can be applied not only to the plasmas but also to general collisionless Boltzmann systems. We must investigate carefully the best fluid model for each problem to be solved.

Acknowledgments

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