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A noise-reducing algorithm for Particle-in-Cell plasma simulation*

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Abstract. In this paper a new algorithm to reduce the noise effects in the Particle-in-Cell method for the Vlasov–Poisson system is proposed. The method is demonstrated on an example of a one-dimensional Riemann problem of plasma physics. Collisionless completely ionized non-isothermic plasma is considered. The model calculates only the ion movement (the electron density is described by the Boltzmann distribution).

1. Introduction

The Particle-in-Cell method (PIC) is widely used to solve plasma problems. It is a Lagrangian method. The positions of a large number of model particles follows the Vlasov kinetic equation characteristics. A particle movement is subject to the law of classical mechanics in the self-consistent electromagnetic field defined from the Maxwell equations [1].

Alternative to the PIC method are grid Vlasov methods. But the latter require large memory and time, especially for three-dimensional problems. Finite difference methods poorly deal with great gradient areas. The Particle-in-Cell method is more efficient, physically intuitive. It is simple and convenient for simulation on parallel computers.

But discreteness of model particles brings about the energy loss, self-force occurrence and other non-physical effects called noise. The reasons for noise occurrence are various [2,3]. Often it is difficult to define the influence of various non-physical factors on the solution as they interact and cooperate with each other.

At the present time, there is no uniform approach to solving the noise problem. More often, the number of particles is increased (that is not always possible because of limitation of computer resources) or the form and distribution of density in a particle are modified [4], or an optimal time and spatial steps are selected. Also, a "quite start" algorithm, Fourier filtering and smoothing algorithms are used (see, e.g., [5, 6]). But such algorithms do not eliminate noise and cut or damp physical effects.

The aim of this work is to develop a noise reducing algorithm, which would not affect a solution (as smoothing algorithms do). At least the

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algorithm is expected only slightly to affect the solution. The algorithm should be general enough for a wide range of problems. The method is demonstrated on an example of one-dimensional Rieman problem of plasma physics.

2. Equations

Collisionless completely ionized non-isothermic plasma was considered, the temperature of electrons greatly exceeding the temperature of ions($T_e \gg T_i$).

The chosen model calculates only the ion movement [7] (without magnetic induction). Electron density is described by the Boltzmann distribution

$$\rho(x) = n_0 \exp\Big(\frac{e\varphi}{T_e}\Big). \tag{1}$$

Only one-dimensional equations are considered. Our system consists of the Vlasov kinetic equation

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial u} = 0, \qquad E = -\frac{\partial \varphi}{\partial x}, \tag{2}$$

and the equation for the electric field potential

$$\beta\frac{\partial^2 \varphi}{\partial x^2} = \exp\varphi - n, \tag{3}$$

where u is the ion velocity, $f(t,x,u)$ is an ion distribution function, $E(t,x)$ is the electric field intensity, $\varphi(t,x)$ is the potential, and $n(t,x) = \int f(t,x,u)\,du$ is the ion density. The potential is measured in T_e/e, the velocity u is measured in $c_s = \sqrt{T_e/m_i}$, $\beta = (D/L)^2$, $D = \sqrt{T_e/4\pi n_0 e^2}$ is the Debye radius, and L is the computation domain length.

3. The Particle-in-Cell scheme

The model particle movement equations are derived from the Vlasov equation by choosing a distribution function in the form [8]:

$$f(t,x,u) = \sum_{j=1}^{m} R(x - x_j(t))\,\delta(u - u_j(t)) \tag{4}$$

where R is a form factor, δ is a delta-function, m is the number of particles,

$$\frac{dx_j(t)}{dt} = u_j(t), \qquad \frac{du_j(t)}{dt} = E(x_j), \qquad j = 1,\ldots,m, \tag{5}$$

are the particles movement equations (characteristics of the Vlasov equation).

In the interval $[0, L]$, the grid with a step h is established, τ is a time step. The time changes from 0 up to $t_{\max}$.

The index i indicates a grid point ($i = 1, \ldots, n$), j is a particle number ($j = 1, \ldots, m$), x_i is coordinate of the ith grid point, x_j^k is the coordinate of the particle j at the time $k\tau$.

Variables φ_i and n_i are set at grid points, E_i is set in the cells centers.

The density and mean velocity are calculated with a distribution function as follows:

$$n(t,x) = \int f(t,x,u)\,du, \qquad v(t,x) = \frac{1}{n(t,x)} \int uf(t,x,u)\,du. \tag{6}$$

For grid functions, this equation is

$$n_i = \sum_{j=1}^{m} R(x_i - x_j), \qquad v_i = \frac{1}{n_i} \sum_{j=1}^{m} u_j R(x_i - x_j). \tag{7}$$

Calculations were conducted with the CIC form factor

$$R(x_i - x_j) = \frac{1}{h} \max\left\{1 - \frac{|x_i - x_j|}{h},\, 0\right\}. \tag{8}$$

One time step of the PIC method consists of the two parts:

Lagrangian step. At this step, from movement equations (5), u_j^{k+1} and x_j^{k+1} at the time $t^{k+1} = (k+1)\tau$ for every particle j are calculated (on the Lagrangian grid):

$$\frac{u_j^{k+1} - u_j^k}{\tau} = E_j^k, \qquad \frac{x_j^{k+1} - x_j^k}{\tau} = u_j^{k+1}.$$

Here E_j^k is the electric field intensity at the point x_j^k where the particle is placed. It is calculated through E_i at grid points.

To pass to the Euler step, the density n_i^{k+1} and mean velocity v_i^{k+1} at the grid points (the Euler grid) x_i are calculated:

$$n_i^{k+1} = \sum_{j=1}^{m} R(x_i - x_j^{k+1}), \qquad v_i^{k+1} = \frac{1}{n_i^{k+1}} \sum_{j=1}^{m} R(x_i - x_j^{k+1}). \tag{9}$$

Euler step. At this step, the nonlinear equation (3) is solved and an electric field is calculated. In this paper, solution to this equation is calculated as follows:

$$\beta \frac{\partial^2 \varphi^{k+1}}{\partial x^2} = \exp(\varphi^{k+1}) - n^{k+1}, \tag{10}$$

where φ^{k+1} is iteratively found from the linear equation

$$\beta\frac{\partial^2\varphi^{k+1,s+1}}{\partial x^2} = \exp(\varphi^{k+1,s})\cdot(1+\varphi^{k+1,s+1}-\varphi^{k+1,s}) - n^{k+1}(x). \qquad (11)$$

In [9], the monotonic convergence of the sequence $\varphi^{k+1,s}$ to solution of equation (10) is shown when $\varphi^{k+1,1} > \varphi^{k+1}$ and, in [10], it is shown that $\varphi^{k+1,1} > \varphi^{k+1}$ with any initial $\varphi^{k+1,0}$.

To pass to the Lagrangian step for the next k, we calculate E_i^{k+1}:

$$E_i^{k+1} = \frac{\varphi_{i-1}^{k+1} - \varphi_i^{k+1}}{h}, \qquad i = 2,\ldots,n.$$

4. Schema of a common noise reducing algorithm

A non-physical fluctuation in velocity leads to discontinuity of a derivative. Although the oscillation amplitude decreases with increasing of the number of particles, these fluctuations bring about electric field fluctuation.

The main idea of the new algorithm is the following:

1. Let us assume the average velocity v^k at time step k to be without noise (without non-physical fluctuations). At the initial moment of time this condition is satisfied because $v|_{t=0} = 0$.
2. The step τ without electric field intensity is done ($E = 0$). Particles, having different velocities, move to new places. The average velocity then appears to have fluctuations, no matter that there was no fields.
3. Denote the noise term by ΔV (it will be defined later). Let us subtract ΔV from velocity of every Particle-in-Cell on time step k, then we have the corrected particles velocity.
4. Now, if the average velocity is calculated again at the step k with formulas (9), it will contain noise. But then, after passing of the step τ, we obtain the average velocity already "without noise" (more correctly, the noise level in the average velocity will be less).

5. The noise term definition

It is known that the Vlasov equation solution is equivalent to that of an infinite system of its moments. In a model of non-isothermic low-density plasma with the Boltzman electron distribution, the ion-sound waves with amplitudes of potential φ smaller than a critical amplitude φ_* ($\varphi < \varphi_* = 1.26$ T/e) can be described [7, 11] by a system consisting of the two first moments of a distribution function and the nonlinear Poisson equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nu) = 0, \qquad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\Big(\frac{1}{2}u^2 + \varphi\Big) = 0, \tag{12}$$

$$\beta \frac{\partial^2 u}{\partial t^2} = 4\pi e\left[n_0 \exp\Big(\frac{e\varphi}{T_e}\Big) - n\right]. \tag{13}$$

Let us call $\widehat{v}^{k+1}$ and $\widehat{n}^{k+1}$ obtained from any finite difference scheme for (12) ($\widehat{v}^k := v^k$, $\widehat{n}^k := n^k$) the "desired" velocity and density. Let us define a noise addition as $\Delta V_i = \widetilde{v}_i^{k+1} - \widehat{v}_i^{k+1}$. It is a difference between the velocity at the time step $k+1$ (at this time step, external field is equal to zero) and the "desired" velocity.

6. A noise subtraction algorithm

1. At the step k, the mean velocity is assumed to be without non-physical fluctuations. At the initial moment of time, this condition is satisfied because $v|_{t=0} = 0$.

2.1. The mean velocity (when $E = 0$) has to satisfy the equation of transport

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}\Big(\frac{1}{2}v^2\Big) = 0, \tag{14}$$

and the density has to satisfy the continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nv) = 0. \tag{15}$$

Obtain $\widetilde{n}^{k+1}$ and $\widetilde{v}^{k+1}$.

2.2. Particle position is adjusted at the time step k in order to $\widetilde{n}^{k+1}$ and $\widehat{n}^{k+1}$ be equal (see below for details).

2.3. The time step τ is done without external fields (electric field intensity in our case). Let us calculate the mean velocity $\widetilde{v}^{k+1}$ and the density $\widetilde{n}^{k+1}$. If $\max\limits_i |\widetilde{v}_i^{k+1} - \widehat{v}_i^{k+1}| < \varepsilon$, then go to Step 4.

3. Define the noise term $\Delta V_i = \widetilde{v}_i^{k+1} - \widehat{v}_i^{k+1}$. Subtracting ΔV_i from every particle velocity in the mesh interval i at the time step k, obtain the adjusted particle velocity:

$$u_j^k := u_j^k - \Delta V_i, \quad x_j \in [(i-3/2)h, (i-1/2)h].$$

Go to Step 2.3.

4. Now the step τ is done with E; obtain v^{k+1}.

7. Particle coordinates adjustment

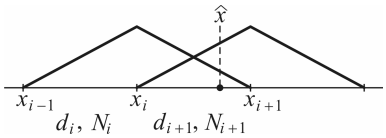

Figure 1. A particle $\widehat{x}$ in the cell a_{i+1}

Let ith mesh interval be denoted as $a_i = [x_{i-1}, x_i]$; N_i be the number of particles in the mesh interval a_i; d_i be the shift for particles in the mesh interval a_i; and $\widehat{x} := x_j$ be a particle (Figure 1).

Particles from the mesh interval a_{i+1} make such a deposition to the density at the ith mesh point

$$n'_i = \frac{m}{h} \sum_{\widehat{x} \in a_{i+1}} (x_{i+1} - \widehat{x}),$$

where m is the mass of one particle.

The density after the shift is

$$n''_i = \frac{m}{h} \sum_{\widehat{x} \in a_{i+1}} (x_{i+1} - \widehat{x} - d_{i+1}).$$

For all particles from the left interval a_i, the density is as follows:

$$n'_{i-1} = \frac{m}{h} \sum_{\widehat{x} \in a_i} (\widehat{x} - x_{i-1}), \qquad n''_{i-1} = \frac{m}{h} \sum_{\widehat{x} \in a_i} (\widehat{x} + d_i - x_{i-1}).$$

The coordinate of a particle $\widehat{x} \in a_i$ after the shift is $\widehat{x}' = \widehat{x} + d_i$.

Then the density at the ith mesh point before the shift is

$$n_i = n'_{i-1} + n'_i = \frac{m}{h} \left(\sum_{\widehat{x} \in a_i} (\widehat{x} - x_{i-1}) + \sum_{\widehat{x} \in a_{i+1}} (x_{i+1} - \widehat{x}) \right)$$

and, after the shift, it is

$$n^*_i = n''_{i-1} + n''_i = \frac{m}{h} \left(\sum_{\widehat{x} \in a_i} (\widehat{x} - x_{i-1} + d_i) + \sum_{\widehat{x} \in a_{i+1}} (x_{i+1} - \widehat{x} - d_{i+1}) \right),$$

$$\Delta n_i = n^*_i - n_i = \frac{m}{h} \left(\sum_{\widehat{x} \in a_i} d_i + \sum_{\widehat{x} \in a_{i+1}} (-d_{i+1}) \right) = \frac{m}{h} (N_i d_i - N_{i+1} d_{i+1}).$$

Let us take $n^*_i = \widehat{n}_i$. Then the system of the algebraic equations with unknown quantities d_i is derived:

$$\Delta n_i = \frac{m}{h} (N_i d_i - N_{i+1} d_{i+1}), \qquad i = 2, \ldots, n-1. \tag{16}$$

The matrix of the system is two-diagonal and the system is incomplete. Let us include one more equation into this system

$$\sum_{i=2}^{n} N_i d_i = 0. \tag{17}$$

This means that the mean shift of all particles is equal to zero.

The particle coordinates adjustment algorithm

1. Having x_j^k, $\widetilde{n}_i^{k+1}$, $\widehat{n}_i^{k+1}$, define d_i $(i = 2, \ldots, n)$ from equations (16), (17) with $\Delta n_i = \widehat{n}_i - \widetilde{n}_i$.
2. The particle coordinates are adjusted $x_j'^{\,k} = x_j^k + d_i$, $x_j \in a_i$, then it follows the velocity adjustment.

8. Numerical experiments

The noise reducing algorithm has been tested on the Riemann problem for the ion density.

The initial density is a smooth function:

$$n(0,x) = \begin{cases} C, & x \in [0, x_0 - b], \\ \dfrac{C+1}{2} + \dfrac{C-1}{2} \cos \dfrac{\pi}{2b}(x - (x_0 - b)), & x \in (x_0 - b, x_0 + b), \\ 1, & x \in [x_0 + b, L]. \end{cases}$$

Here C is the density on the left boundary, b is a smoothing factor, $x_0 = L/2$.

The initial condition for the potential is

$$\varphi(x, 0) = \ln n(x). \tag{18}$$

The boundary conditions are chosen equal to the initial condition because the basic movement occurs far sufficiently from the boundaries of the domain

$$\varphi(0, t) = \ln C, \qquad \varphi(L, t) = 0. \tag{19}$$

The particle distribution function is a Maxwell one. The mean velocity equals to 0 and the dispersion (temperature) equals to 0.05. In all the tests, the "quite start" algorithm was used.

The following parameter values are used in the experiments: $L = 4$, $b = 0.1$, $C = 2$. The time interval is $t_{\max} = 0.3$ and the time step is $\tau = 0.001$. The Particle-in-Cell method parameters: the number of particles is $m = 6000$ and the number of grid points is $n = 101$.

A usual Particle-in-Cell solution method without reducing a noise using the predictor-corrector scheme for (14), (15) was compared with the Lax–Vendroff solution of the Vlasov equation.

A selected scheme for calculation $\widehat{v}$ and $\widehat{n}$ affects the solution. Three schemes for solving (14), (15) were tested — the upwind difference scheme,

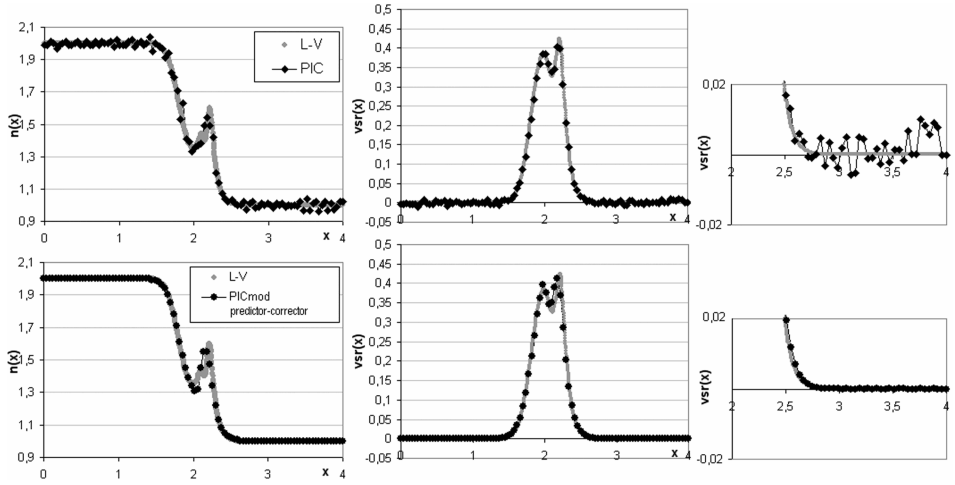

Figure 2. Comparison of density and mean velocity

the Lax–Vendroff, and the predictor-corrector. Finally, the predictor-corrector scheme was chosen.

In Figure 2, a density and a mean velocity for the usual Particle-in-Cell method (PIC, black markers in the figures above) and for the modified Particle-in-Cell method (PICmod predictor-corrector, black markers in the figures below) are compared with the Lax–Vendroff solution (the gray line). The last two figures on the right represent a detailed view of the mean velocity function.

In this figure, the presence of noise is evident in the average velocity and density evaluated by the PIC method. The modified PIC algorithm allows us to reduce a noise level in the areas $A := [0, 1]$ and $B := [3, 4]$.

The disturbance has not reached the regions A and B yet, so the mean velocity is equal to zero here; the density is equal to 2 on the left and to 1 on the right. Thus, the noise rate can be numerically estimated. We introduce the noise magnitudes for the density and the mean velocity in the areas A and B:

$$\Delta v = \sum_{ih \in A \cup B} |v_i|, \qquad \Delta n = \sum_{ih \in A} |2 - n_i| + \sum_{ih \in B} |1 - n_i|.$$

In the table, the noise magnitudes for the usual and modified Particle-in-Cell methods are compared. The number of grid points is 101, time is 0.1, time step is 0.001.

It is evident that the modified Particle-in-Cell method noise magnitude is lower than the usual one.

The dependence of the noise magnitude for PIC and PICmod methods

Noise magnitude	Number of particles			
	5000	10000	40000	60000
Δn, PIC	$4.99 \cdot 10^5$	$2.28 \cdot 10^5$	$1.74 \cdot 10^5$	$1.51 \cdot 10^5$
Δn, PICmod	$1.37 \cdot 10^2$	$7.88 \cdot 10^3$	$4.57 \cdot 10^3$	$3.01 \cdot 10^3$
Δv, PIC	$1.82 \cdot 10^5$	$5.86 \cdot 10^6$	$3.16 \cdot 10^6$	$2.71 \cdot 10^6$
Δv, PICmod	$2.27 \cdot 10^3$	$7.88 \cdot 10^3$	$1.06 \cdot 10^3$	$5.18 \cdot 10^4$

9. Conclusion

A new noise reducing algorithm for the Particle-in-Cell method is presented. The conducted testing of this algorithm has shown its availability. The given algorithm really allows one to reduce noise in the mean velocity and density in the particles-in-cell method for foregoing problem. The solution quality depends on a choice of scheme choice at Step 2.1 of the noise subtraction algorithm.

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