EFFECTS OF SPATIAL GRID
IN PLASMA SIMULATIONS
USING HIGHER ORDER MULTIPOLE EXPANSIONS

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Printed in the United States of America.

Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

Price: Printed Copy \$ * ; Microfiche \$3.00

<u>*Pages</u>	<u>NTIS Selling Price</u>
1-50	\$ 4.00
51-150	5.45
151-325	7.60
326-500	10.60
501-1000	13.60

Effects of Spatial Grid in Plasma Simulations*

Using Higher Order Multipole Expansions

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PPPL-1355

July 1977

ABSTRACT

Reduction of nonphysical grid effects in plasma simulations has been examined numerically using higher order multipole expansions in one dimension. It is found that keeping the higher order moments, such as quadrupole and octapole moments, substantially reduces the grid effects for small Debye length so that the numerical results agree well with the predictions from the gridless theory. In particular, it is found that the grid instabilities for small Debye length diminish when the higher order moments are used.

1. INTRODUCTION

The use of spatial grid in plasma simulations using finite size particles has been widespread and physical as well as nonphysical properties of such methods have been studied in detail [1-4]. Methods such as Particle-in-Cell (PIC), Cloud-in-Cell (CIC), and dipole expansion methods are commonly employed for simulating collisionless plasmas using finite-size particles [5-7].

When a spatial grid is introduced for the simulation of plasmas together with the fast Fourier transform algorithm, not only the phenomena having the short wavelength ($k > \pi/\Delta$) in comparison with the grid size, Δ , are lost, but the phenomena with the wavelength longer than the grid size ($k \leq \pi/\Delta$) are also modified. When the Debye length is small in comparison with Δ , it is known that all the above-mentioned methods suffer from numerical instabilities [3, 8, 9]. While the use of finite-size particles already modifies the fundamental plasma properties from the real ones, it appears that one cannot do much about this so long as one aims at simulating real plasmas using a far fewer number of particles. Modifications are significant, however, only for the short wavelength modes.

While the use of finite-size particles is inevitable in two and three dimensional simulations, one should, in principle, use the smallest size of particles to reduce the modification of physics and at the same time increase the number of simulation

particles as much as one can afford so that the noise and collisions do not destroy the physics one is trying to simulate.

In practice, the size of particles, a , is taken about the Debye length, λ_D , for most of the simulations since one is not interested in phenomena having the wavelength shorter than the Debye length and, therefore, such phenomena can be suppressed in numerical simulations. The Debye length in turn can be taken smaller than the grid size when one is interested in the physics at very long wavelength compared with the Debye length. For such a case, both the particle size and the Debye length are smaller than the grid size and it is under such situations that the above-mentioned numerical methods, such as PIC, CIC, and dipole methods, become poor approximations.

In the next Section, we compare the numerical results for the thermal fluctuations obtained from the higher order multipole expansion method with the theoretical predictions. It is found that keeping the higher order moments, such as quadrupole and octapole moments, substantially improve the simulation results even for small Debye length and particle size.

2. NUMERICAL RESULTS

As an example for testing the numerical method using higher order moments, we consider a one-dimensional electron plasma model in the electrostatic limit. The ions are assumed immobile

background. Initially, electrons are more or less uniform in space and the velocity distribution is close to a Maxwell distribution. For such a plasma, one can use equilibrium plasma theory to predict thermal fluctuations given by [1]

$$\frac{LE_k^2}{4\pi T_e} = \frac{1}{1 + k^2 \lambda_D^2 \exp(k^2 a^2)} \quad (1)$$

where $L = 64 \Delta$ is the system length, T_e is the electron temperature, a is the size of a gaussian particle defined by the form factor

$$S(x) = \frac{1}{\sqrt{2\pi}a} \exp(-x^2/2a^2) \quad (2)$$

Equation (1) is for the gridless case and the grid effect is given in Ref. 4. Our interest here is to recover the gridless results in the simulations. $\omega_{pe} \Delta t = 0.2$ is used for all the runs reported here.

In the examples given below, moments up to octapoles are examined using the multipole expansion method. In this method, Poisson's equation is written in k space and then the charge density is expanded around the nearest grid point keeping up to the desired moments. They are given by

$$\begin{aligned}
 k^2 \phi_k &= 4\pi \sum_j q_j \exp(-k^2 a^2/2) \exp(-ik\delta x_j) \\
 &= 4\pi q \exp(-k^2 a^2/2) \sum_j \left(1 - ik\delta x_j - \frac{(k\delta x_j)^2}{2!} + \frac{i(k\delta x_j)^3}{3!} \dots \right) \\
 &= 4\pi q \exp(-k^2 a^2/2) \sum_{s=1}^L \left(g_0^s - ikg_1^s - k^2 g_2^s + ik^3 g_3^s + \dots \right)
 \end{aligned} \tag{3}$$

where

$$\begin{aligned}
 g_0^s &= \sum_{j \in s} 1 \\
 g_1^s &= \sum_{j \in s} \delta x_j \\
 g_2^s &= \sum_{j \in s} (\delta x_j)^2/2!
 \end{aligned} \tag{4}$$

and

$$g_3^s = \sum_{j \in s} (\delta x_j)^3/3!$$

Here $\delta x_j = x_j - s\Delta$ is the displacement of the j th particle from the nearest grid point, s , and g_0^s , g_1^s , g_2^s , and g_3^s are the.

moments associated with the grid point. $k = 2\pi m/L$ where $m = 0, 1, 2, \dots, L-1$ and q is the total charge of an electron.

The force on the j th particle is calculated similarly. It is given by

$$F(x_j) = \frac{q_j}{\sqrt{2\pi} a} \sum_{m=0}^{L-1} \exp(-k_m^2 a^2/2) E_{km} \exp(ik_m \Delta) \left(1 + ik_m \delta x_j - \frac{(k_m \delta x_j)^2}{2!} - \frac{(k_m \delta x_j)^3}{3!} + \dots \right) \quad (5)$$

In the following, four different values of the Debye length are compared with theoretical predictions using dipole (DP), quadrupole (QP), and octapole (OP) moment expansions using various size of particles. The first case is $\lambda_D/\Delta = 1$ and $a/\Delta = 1$ and 0.5. The second case is $\lambda_D/\Delta = 0.5$ and $a/\Delta = 0.5$ and 0.25. Then $\lambda_D/\Delta = 0.25$ and $a/\Delta = 0.5$ and 0.25 are examined for the case 3. The last case is $\lambda_D/\Delta = 0.1$ and $a/\Delta = 0.5$.

1. Case 1

$$\lambda_D/\Delta = 1 \text{ and } a/\Delta = 1, 0.5$$

The first example is the case with the Debye length equal to the grid size, typically used for many plasma simulations. The particle size is chosen 1 and 0.5 and the results are shown in Figs. 1(a) and (b). Note all the results for the fluctuation spectrum reported here are averaged in time from $\omega_{pe} t = 0$ and $\omega_{pe} t = 250$.

For $a = \Delta$, we observe all the three methods (DP, QP, and OP) agree very well with the gridless theory given by Eq. (1). Note the wavelength for this case is given by

$$k_m \lambda_D = 2\pi m / 64 = 0.1 \text{ m} .$$

For $m \geq 10$ ($k\lambda_D \geq 1$) , the finite size particle greatly suppresses the short wavelength mode. The modification due to the use of finite-size particles from the zero-size particles is already significant for $m = 10$ ($k\lambda_D = 1$) .

To make the modification smaller, $a/\Delta = 0.5$ is tested in Fig. 1(b). We observe all the three methods agree very well with the theory for $m \leq 20$ ($k\lambda_D \leq 2$) . Systematic enhancement is clearly seen for the dipole method for $20 \leq m \leq 32$ while the higher order moment methods (QP, OP) agree well with the gridless theory up to the last mode ($m = 32$) .

In practice, one is not generally interested in the modes with $k\lambda_D \geq 1$, the dipole method works satisfactorily for both $a/\Delta = 1$ and 0.5 ; it is probably unnecessary to use higher order expansions for this case.

2. Case 2

$$\lambda_D/\Delta = 0.5 \text{ and } a/\Delta = 0.5 , 0.25$$

Figure 2(a) corresponds to the case with $\lambda_D/\Delta = 0.5$ and $a/\Delta = 0.5$ so that

$$k_m \lambda_D = \pi m / 64 \approx 0.05 m$$

for this case. We observe again that for $m \lesssim 20$ ($k \lambda_D \lesssim 1$) all the methods agree quite well with the theory except for small m modes such that

$$m \lesssim 6 \quad (k \lambda_D \lesssim 0.3) .$$

This is apparently due to the fact that the Landau damping rate is so weak for these modes that they have not reached the thermal equilibrium during the course of computations.

Landau damping rate for a one-dimensional plasma model is given by

$$\frac{\gamma}{\omega_{pe}} = \frac{1}{2} \left(\frac{\pi}{2} \right)^{1/2} \frac{1}{k^3 \lambda_D^3} \exp \left(- \frac{1}{2k^2 \lambda_D^2} - \frac{3}{2} \right) \quad (6)$$

which gives $\gamma \approx 10^{-4} \omega_{pe}$ for $k \lambda_D = 0.2$ which is too small compared with the running time. Note that the collisional relaxation is also very small for a one-dimensional plasma [10].

For $m \gtrsim 20$ ($k \lambda_D \gtrsim 1$), the dipole moment method deviates from the theory while quadrupole and octapole moments are in good agreement up to the last mode. The modification due to the use of finite-size particle is considerably smaller here

compared with Case 1 and as long as the long wavelength modes ($k\lambda_D \lesssim 1$) are concerned, the dipole moment gives satisfactory results.

When the particle size is further reduced to $a/\Delta = 0.25$, we observe that the dipole and quadrupole moment methods indicate a systematic deviation for $m \gtrsim 20$ ($k\lambda_D \gtrsim 1$) and $m \gtrsim 25$ ($k\lambda_D \gtrsim 1.25$) while the octapole moment method follows the theory up to the last mode. Note that the size of a particle is small enough so that the modifications from the zero-size particle is quite small for the long wavelength modes ($k\lambda_D \lesssim 1$).

3. Case 3

$$\lambda_D/\Delta = 0.25 \text{ and } a/\Delta = 0.5, 0.25$$

Figures 3(a) and (b) correspond to a small Debye length $\lambda_D/\Delta = 0.25$ so that the mode for the system is

$$k_m \lambda_D = \pi m / 128 \approx 0.025 m.$$

Since the wavelength is very small for small m , more and more modes in the long wavelength ($m \lesssim 10$) is under thermal level because the equilibration time for them is just too long.

For the case of $a/\Delta = 0.5$, again the quadrupole and octapole moment methods show good agreement for the entire range while the dipole scheme shows the enhancement for the higher mode number.

For the case of $a/\Delta = 0.25$, the quadrupole and octapole moment methods agree well with theory which is very close to the zero-size particle result for the entire region in k space. The dipole moment method indicates systematically higher fluctuations for most of the modes. For the parameters chosen here, it is clear one has to use either quadrupole or octapole moment methods which then give essentially gridless results with little modifications due to the use of finite-size particles.

4. Case 4

$$\lambda_D/\Delta = 0.1 \text{ and } a/\Delta = 0.5$$

This is the case of a small Debye length where the conventional methods such as CIC, PIC, and DP are all unstable against the numerical instabilities due to aliases. The mode for this case is given by

$$k_m \lambda_D = \pi m / 320 \approx 0.01 m.$$

Figure 4(a) is the total energy with time for three methods (DP, QP, and OP). We see the dipole scheme is quite unstable increasing the total energy by 18% until $\omega_{pe} t = 250$. The quadrupole method reduces the growth rate, but it is still unstable. The octapole scheme completely stabilizes the numerical instability and we find the energy is conserved within one part in 10^4 for the entire run.

Figure 4(b) indicates the time-averaged spectrum for the octapole scheme. Good agreement is found for the short wavelength mode $m \gtrsim 20$ ($k\lambda_D \gtrsim 0.2$) while the long wavelength modes $m \lesssim 20$ ($k\lambda_D \lesssim 0.2$) are largely under thermal noise because of their long equilibration time.

3. DISCUSSIONS AND CONCLUSIONS

We have examined the higher order multipole moment method by comparing the thermal fluctuations with the predictions from the gridless theory with and without using finite-size particles. We find:

(a) For $\lambda_D/\Delta = a/\Delta = 1$ which is commonly used for plasma simulations, all the three methods (DP, QP, and OP) agree well with the gridless theory. For $\lambda_D/\Delta = 1$ and $a/\Delta = 0.5$, the dipole scheme shows the enhancement for $k\lambda_D \geq 2$ while the quadrupole and octapole schemes agree up to the last mode. Furthermore, modifications due to the use of finite-size particles is small for long wavelength modes ($k\lambda_D \lesssim 1$).

(b) For $\lambda_D/\Delta = 0.5$, all the schemes give good agreement for $k\lambda_D \lesssim 1$ while the dipole scheme gives enhanced noise for $k\lambda_D \geq 1$. The quadrupole and octapole schemes agree well for the entire modes.

(c) For $\lambda_D/\Delta = 0.25$, the dipole scheme gives enhanced fluctuations for the wide range of spectrums while the quadrupole and octapole schemes again give good agreement with theory.

(d) For $\lambda_D/\Delta = 0.1$, the quadrupole scheme is stable against the numerical instabilities, and the spectrum is also in good agreement with the theoretical predictions.

While the dipole scheme is good enough for most of the simulations, it is sometimes necessary to use higher order moments especially when one is interested in obtaining the results free from spatial grid and modifications due to the use of finite-size particles. Obviously, the higher order moment method is more costly and requires more computer memories, especially in multidimensional simulations, but it gives much better physical results. The data presented here should provide some guidance as to the choice of numerical method.

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Fig. 1. Time averaged ($\omega_{pe} t = 0 - 250$) fluctuation spectrum for $\lambda_D/\Delta = 1$ using dipole (DP), quadrupole (QP), and octapole (OP) moment methods. Solid lines are theoretical predictions. $a/\Delta = 1$ (a) and $a/\Delta = 0.5$ (b).

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 Fig. 2. Time-averaged spectrum for $\lambda_D/\Delta = 0.5$ and $a/\Delta =$
 0.5 (a) and $a/\Delta = 0.25$ (b).

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Fig. 3. Time-averaged spectrum for $\lambda_D/\Delta = 0.25$ and $a/\Delta = 0.5$ (a) and $a/\Delta = 0.25$ (b).

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Fig. 4. Time history of the total energy for DP, QP, and OP schemes (a), and the time-averaged spectrum for the OP scheme (b). $\lambda_D/\Delta = 0.1$ and $a/\Delta = 0.5$.