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ELECTROSTATIC AND MAGNETOSTATIC
PARTICLE SIMULATION MODELS
IN THREE DIMENSIONS

BY

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PLASMA PHYSICS
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Electrostatic and Magnetostatic Particle Simulation
Models in Three Dimensions

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ABSTRACT

Electrostatic and magnetostatic particle simulation models have been developed and tested for a magnetically confined plasma near thermal equilibrium. The model makes use of a three-dimensional grid elongated in the direction of a magnetic field to simulate plasma confinement devices. Linear interpolation is used on a two-dimensional grid perpendicular to a magnetic field while quadratic or cubic interpolation is used in the direction of the magnetic field. It is found that the energy conservation is good and the fluctuation spectra for the electric and magnetic fields agree with theoretical predictions. The model presented here may be used as an alternative method to simulate a laboratory device along with the hybrid model which makes use of the combination of a two-dimensional spatial grid and an eigenfunction expansion along the main magnetic field.

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I. INTRODUCTION

The use of plasma simulation techniques for understanding the complex plasma behavior has been established along with the advancement in large-scale scientific computers and the numerical techniques which can handle such systems. Quite a few models have been developed depending on the problems concerned. Particle simulation models, magnetohydrodynamic models, kinetic models, and transport models are some of these examples [1].

For simulating microscopic processes in a magnetically confined plasma, particle simulation models become essential. In particular, plasma turbulence in a magnetically confined plasma may be highly nonlinear and complex involving anomalous transport and ergodic magnetic field lines. Under such conditions, it is essential to have full three-dimensional simulation models available to understand the physical processes involved [2]. Such models have been constructed for both cylindrical and toroidal systems using a two-dimensional grid for the plasma cross section and the eigenfunction expansions in the axial direction [3]. It is shown that the model is quite useful for the study of anomalous diffusion due to electrostatic drift and trapped-particle turbulence in both the cylindrical and toroidal systems. The reason for that is that, while the plasma in a confining magnetic field is long compared with their transverse dimensions, one can discard the

short wavelength fluctuations along the field lines while keeping several important long wavelength modes. This is done most conveniently by expanding the field quantities in terms of eigenfunctions along the magnetic field while a two-dimensional spatial grid may be used in a plane perpendicular to the field. This method is accurate and fast enough when the modes kept in the axial direction are, say, 10 or so. When it becomes necessary to include more modes in the axial direction, then it will be advantageous to introduce a spatial grid in the direction of the magnetic field along with the other two directions. This method will probably reduce the computing time compared with the eigenfunction expansion method, provided many modes (10 or more) are required. It is obvious, however, this approach is less accurate since the physical quantities are defined only on discrete grid points along the magnetic field. Furthermore, it is important to avoid the numerical instabilities which may arise when a coarse grid is used in the simulation [4].

In this paper, we develop both electrostatic and magneto-static models in a cylindrical geometry using a three-dimensional grid and test them for a plasma near thermal equilibrium. Since the physical system we are modeling is long compared with the cross section, an elongated grid is necessary in the axial direction compared with the grid in the cross section. It is, therefore, necessary to use higher order interpolations in the axial directions such as quadratic, cubic splines, or even a

higher order scheme using gaussian interpolations [5, 6, 7]. For the cross section, linear interpolation or dipole approximation is usually sufficient. In Section II, an electrostatic model is developed and the result for the thermal spectrum is compared with theoretical expectations. A magnetostatic model which is appropriate for a low β plasma ($\beta \equiv$ plasma pressure/magnetic pressure) is also developed and tested in Section III. Concluding remarks are given in Section IV.

II. ELECTROSTATIC MODEL

Let us first consider an electrostatic model in a three-dimensional rectangular box in a magnetic field which is taken in z direction. The system is elongated along the magnetic field so that $L_z \gg L_x, L_y$ where L_x, L_y , and L_z are the length of the system in three directions. Following the conventional procedure, a spatial grid is introduced to solve Poisson's equation and to push particles. Since $L_z \gg L_{x,y}$, the grid size in z will be much larger than the grid size in x and y . This is because we do not want to keep short wavelength fluctuations in that direction. Keeping the short wavelength modes will require much more computer memory and more particles and it is of no interest for the present model. The number of grid points in z depends on how many modes are physically required in the axial direction. While the physical

length of the system is much longer than the cross section, the number of important modes along the field is ordinarily not more than the number in the cross section when studying the low frequency plasma turbulence and anomalous plasma diffusion ($k_{\perp} \gg k_{\parallel}$).

Since the grid size in z (Δz) is usually much larger than the plasma Debye length, it is desirable to use an interpolation scheme higher than the linear interpolation or dipole expansion method. One would not like to go too high at the same time since the limited computing time will make such a scheme impractical. If the system remains numerically unstable, one has, of course, no choice but to use a higher order scheme or to change the simulation parameters. Here we test quadratic and cubic splines in z direction and linear interpolations in $x - y$ plane. Higher order interpolations such as gaussian interpolations do not seem necessary for the cases tested although they should give better results at the sacrifice of computing time [5].

The first example (case 1) is the following: $16 \times 16 \times 16$ grid in (x, y, z) , $16 \times 16 \times 160$ Debye length system in (x, y, z) , $a_x/\Delta x = a_y/\Delta y = 1$ and $a_z/\Delta z = 1$ (a_x, a_y, a_z are the width of the gaussian particles used and $\Delta x, \Delta y, \Delta z$ are the grid size), $m_i/m_e = 25$, $T_e/T_i = 1$, $\omega_{pe}/\Omega_e = 1$, $\omega_{pe}\Delta t = 0.2$, and the total number of particles = 4096 are used. The system is triply periodic and the plasma is uniform. Quadratic splines are used in the z direction. Note the grid size in z is 10 times larger than Δx and Δy . Figure 1 shows the time

averaged fluctuation spectra for the electric field. Both the two-dimensional modes $\underline{k} = (k_x, k_y, 0)$ and the one-dimensional modes $\underline{k} = (0, 0, k_z)$ are shown to detect the grid effects. Both measurements agree very well with theoretical fluctuations shown by the solid lines given by

$$\frac{V(E_k)^2}{8\pi} = \frac{T}{2} \frac{1}{1 + k^2 \lambda_D^2 S^{-2}(k)} \quad (1)$$

where

$$S^2(k) = \exp[-(k_x^2 a_x^2 + k_y^2 a_y^2 + k_z^2 a_z^2)]$$

$$\cdot \left(\frac{\sin(k_x \Delta x/2)}{k_x \Delta x/2} \right)^4 \left(\frac{\sin(k_y \Delta y/2)}{k_y \Delta y/2} \right)^4 \left(\frac{\sin(k_z \Delta z/2)}{k_z \Delta z/2} \right)^6 \quad (2)$$

is the effective shape factor for the gaussian particles averaged over the spatial grid using the linear and quadratic interpolations and V is the plasma volume [8, 9]. There is no apparent sign for the numerical grid instabilities even for the one-dimensional modes propagating along the magnetic field [5]. This is because the instability is rather weak for this case and the number of such one-dimensional modes are very small compared with the total number of modes available. The total energy conservation was 0.08 percent for the entire length of the run (2000 steps). This is surprisingly good

considering the fact that there is only one particle per grid and the very large physical volume of the simulation plasma.

Figure 2 indicates the temporal behavior of the electric field energies in three directions. There is no apparent sign of growth and they oscillate around the mean value. Note $\langle E_z^2 \rangle \ll \langle E_x^2 \rangle, \langle E_y^2 \rangle$ since $L_z \gg L_x$ and L_y .

One can improve the total energy conservation significantly by discarding the one-dimensional modes $\underline{k} = (0, 0, k_z)$ at the step when pushing particles, since the one-dimensional modes may be subject more easily to numerical grid instabilities. When this is done (case 2), the total energy conservation is 0.04% for the same length of run. Figures 3 and 4 indicate the time averaged spectrum and the temporal behavior of the electric field fluctuations. The agreement of the measured fluctuations with theory is again excellent. Temporal behavior is about the same as Fig. 2 for the electric field components across the magnetic field, $\langle E_x^2 \rangle, \langle E_y^2 \rangle$, while $\langle E_z^2 \rangle$ is smaller. This is partly because of the obvious reason that the one-dimensional modes (16 modes) are missing here and partly because these modes may be weakly unstable which tends to enhance the fluctuations along the magnetic field.

When the system is further elongated along the magnetic field to a $16 \times 16 \times 320$ system while keeping all the other parameters unchanged, it is observed that the one-dimensional modes $\underline{k} = (0, 0, k_z)$ become slightly unstable in accordance with the numerical instability for the quadratic interpolations [5].

The overall energy conservation as well as the fluctuation spectra are again in good agreement with theory. One can again discard the weakly unstable one-dimensional modes since they are not important at all as far as the plasma confinement physics is concerned.

The same examples are also tested by using cubic splines in z while keeping linear interpolations in $x - y$ plane. While the results are certainly improved with no signs of numerical instabilities, the overall difference is not much. The total energy conservation is, for example, 0.04% or so for 2000 steps of iteration for both examples. This is because the quadratic spline is already good enough for the examples considered. As will be shown later, more difference is observed for the magnetostatic model in which a nonlinear equation has to be solved.

III. MAGNETOSTATIC MODEL

Let us now develop a magnetostatic model appropriate for a low β ($\beta \ll 1$) plasma [10]. Using the same configuration as previously used, only the x, y components of the self-consistent magnetic field, B_x, B_y and the z component of the transverse electric field E_z^T are kept in addition to the longitudinal electric field $E^L = -\nabla\phi$. The perturbed magnetic field in z is neglected since it is much smaller than the external given field B_0 . The x, y components of E^T are also assumed much smaller than E_x^L and E_y^L . These assumptions are generally valid as long as $\beta \ll 1$.

The set of field equations in this model may be written as

$$\nabla \times \underline{B} = \frac{4\pi}{c} \underline{J}^T \quad (3a)$$

$$\nabla \times \underline{E}^T = - \frac{1}{c} \frac{\partial \underline{B}}{\partial t} \quad (3b)$$

$$\nabla^2 \phi = -4\pi\rho$$

$$\underline{E}^L = -\nabla\phi . \quad (3c)$$

$\underline{B}$ is obtained by taking the curl of (3a);

$$\nabla^2 \underline{B} = - \frac{4\pi}{c} \nabla \times \underline{J}$$

or, in k space,

$$\begin{aligned} B_x(k) &= i \frac{4\pi}{ck^2} (k_y J_z - k_z J_y) \approx i \frac{4\pi}{c} \frac{k_y}{k^2} J_z \\ B_y(k) &= i \frac{4\pi}{ck^2} (k_z J_x - k_x J_z) \approx -i \frac{4\pi}{c} \frac{k_x}{k^2} J_z \end{aligned} \quad (4)$$

where only the z component of $\underline{J}$ is kept here since it is much larger than the terms neglected for low frequency oscillations in an elongated system along the main magnetic field ($k_z \ll k$).

To obtain E_z^T , we first take the curl of (3b) to find

$$\nabla^2 \tilde{E}^T = \frac{4\pi}{c^2} \frac{\partial}{\partial t} \tilde{J}^T$$

or, in k space,

$$-k^2 \tilde{E}^T(k) = \frac{4\pi}{c^2} \left. \frac{\partial \tilde{J}}{\partial t} \right|^T. \quad (5)$$

$\partial \tilde{J} / \partial t$ is now replaced by using the equation of motion [11, 12].

$$\begin{aligned} \frac{\partial \tilde{J}}{\partial t} &= \sum_j q_j \left[\frac{q_j}{m_j} \left(\tilde{E} + \frac{1}{c} \tilde{v}_j \times \tilde{B} \right) f(\tilde{r} - \tilde{r}_j) - \tilde{v}_j \tilde{v}_j \cdot \nabla f \right] \\ &= \frac{q^2}{m_e} \left(n \tilde{E} + \frac{1}{c} \tilde{J} \times \tilde{B} \right) - \sum_j q_j \tilde{v}_j \tilde{v}_j \cdot \nabla f \end{aligned}$$

where $n = n_e + (m_e/m_i) n_i$ and $\tilde{J} = \tilde{J}_e + (m_e/m_i) \tilde{J}_i$. Equation (5) becomes now

$$-k^2 \tilde{E}^T = \frac{4\pi q^2}{m_e c^2} (n \tilde{E})^T + \left(\frac{4\pi q^2}{m_e c^2} \frac{\tilde{J} \times \tilde{B}}{c} - \frac{4\pi}{c} \sum_j q_j \tilde{v}_j \tilde{v}_j \cdot \nabla f \right)^T \equiv \tilde{S}^T.$$

Writing $n = n_0 + \delta n$, and taking the z component of the above equation, we find

$$-\left[k^2 + \frac{\omega_{pe}^2}{c^2} \left(1 + \frac{m_e}{m_i}\right) \exp(-k^2 a^2)\right] E_z^T = \frac{4\pi q^2}{m_e c^2} (\delta n_e)_z^T + S_z^T \quad (6)$$

where

$$(\delta n_e)_z^T = \left(1 - \frac{k_z^2}{k^2}\right) (\delta n_e)_z - \frac{k_x k_z (\delta n_e_x^L) + k_y k_z (\delta n_e_y^L)}{k^2} \quad (7)$$

Note in Eq. (6), (δn_e) is first calculated by multiplying δn and E in real space and then transformed into k space. Note also $E_{x,y}^T$ are neglected since they are assumed much smaller than $F_{x,y}^L$. Equation (6) is solved by iteration. First, $(\delta n_e)_z^T$ in Eq. (7) is neglected and we find

$$E_{z0}^T = -\left(-\frac{4\pi q^2}{m_e c^2} \frac{k_x k_z (\delta n_e_x^L) + k_y k_z (\delta n_e_y^L)}{k^2} + S_z^T\right)$$

$$\cdot \left[k^2 + \frac{\omega_{pe}^2}{c^2} \left(1 + \frac{m_e}{m_i}\right) \exp(-k^2 a^2)\right]^{-1}.$$

Then the corrected value of E_z^T is found by using E_{z0}^T in Eqs. (6) and (7).

Figures 5 and 6 show the time averaged magnetic field fluctuations for the two-dimensional ($k_z = 0$) and three-dimensional modes ($k_z = 2\pi/L_z$) using quadratic splines. Note the agreement with theoretical prediction given by

$$\frac{V(B_k)^2}{8\pi} = \frac{T}{2} \frac{1}{1 + (k^2 c^2 / \omega_{pe}^2) S^{-2}(k)} \quad (8)$$

is very good. The parameters for the simulation (case 3) are $16 \times 16 \times 16$ grid and particles in (x, y, z) , $16 \times 16 \times 160$ Debye length system in (x, y, z) , $a_x/\Delta x = a_y/\Delta y = a_z/\Delta z \approx 1$, $m_i/m_e = 25$, $T_e/T_i = 1$, $\Omega_e/\omega_{pe} \approx 2$, $c/v_e = 5$ and $\omega_{pe} \Delta t = 0.2$. The system is triply periodic and uniform. Note the plasma β is 4% here. Frequency spectra for the magnetic field fluctuations for this case reveal that the two-dimensional modes are zero frequency while the shear Alfvén waves correspond to the three-dimensional modes. The frequencies agree with linear theory. Needless to say, the electrostatic fluctuation spectra also agree very well with theory. The total energy conservation is about 1% at the end of the run (1000 steps) which was much worse compared with that for the electrostatic model. In fact the model appears to be slightly unstable for the parameters chosen. When cubic interpolation is employed in z direction, the total energy conservation was better than 0.05% for the same length of the run, as good as that for the electrostatic model and the system remains completely stable. Therefore, the non-linear equation for E_z^T , Eq. (6) appears to be subject to numerical aliases more than the linear equations. For both cases, collective behavior of plasmas, such as fluctuation spectra, agree well with the theoretical prediction shown in Figs. 5 and 6.

IV. DISCUSSIONS AND CONCLUSIONS

We have developed electrostatic and magnetostatic particle simulation models in three dimensions using a three-dimensional spatial grid elongated along the main magnetic field. Linear interpolation was used in the two-dimensional plane perpendicular to the main magnetic field while quadratic or cubic interpolation was employed in the direction of the magnetic field. Both models behave properly and the fluctuation spectra for electric and magnetic fields agree very well with theoretical predictions. In particular, cubic splines give much better results for the magnetostatic model. No apparent sign of numerical grid instabilities have been detected except for the one-dimensional electron plasma waves propagating along the magnetic field which can be eliminated in the equation of motion as discussed. For the case of quadratic or cubic interpolation, however, the growth rate of the Maxwellian plasmas remains small [5]. While no detail work exists for the numerical solution of the grid instabilities for the oblique plasma waves, it is apparent that the growth rates of the instabilities are very small since the frequency itself is small, $\omega \sim \omega_{pe} k_{||}/k \ll \omega_{pe}$, in comparison with the plasma frequency. In particular, the use of cubic interpolations eliminates the possible numerical instabilities [5]. Some more work is necessary for determining the growth rate for the numerical instabilities [13].

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FIGURE CAPTIONS

Fig. 1. Time averaged electric field fluctuation spectra for the two-dimensional, $\underline{k} = (k_x, k_y, 0)$, and one-dimensional, $k = (0, 0, k_z)$, modes averaged over the entire length of the run ($\omega_{pe} t = 0 - 400$). Case 1.

Fig. 2. Temporal behavior of the electric field fluctuations along and across the magnetic field. Note there is no apparent sign of temporal growth. Case 1.

Fig. 3. Time averaged electric field fluctuation spectra for the case where the one-dimensional modes $\underline{k} = (0, 0, k_z)$ are discarded. Case 2.

Fig. 4. Temporal behavior of the electric field fluctuations along and across the magnetic field. Case 2.

Fig. 5. Time averaged magnetic field fluctuations for the two-dimensional modes, $\underline{k} = (k_x, k_y, 0)$, averaged over the entire length of the run ($\omega_{pe} t = 0 - 200$). Case 3.

Fig. 6. Time averaged magnetic field fluctuations for the three-dimensional modes, $\underline{k} = (k_x, k_y, k_z = \pm 2\pi/L_z)$ averaged over the entire length of the run. Case 3.

Fig. 1. 782173

Fig. 2. 782170

Fig. 3. 782174

Fig. 4. 782169

Fig. 5. 782171

Fig. 6. 782168