NEW THREE-DIMENSIONAL SIMULATION
MODELS FOR CYLINDRICAL AND
TOROIDAL PLASMAS

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New Three-Dimensional Simulation Models
for Cylindrical and Toroidal Plasmas

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A new class of three-dimensional particle simulation models using finite-size particles has been developed which is useful for studying plasma behavior in large, cylindrical and toroidal systems. The model makes use of the combination of eigenfunction expansion and the multi-pole expansion on a two-dimensional spatial grid for solving the Maxwell Equations and for pushing particles. For a toroidal system, the Poisson equation is solved by using the cubic spline technique in the radial direction. It is shown that full three-dimensional simulations may be carried out for real plasma devices such as tokamaks or pinch devices using the presently available computers. Results of the simulations for the thermal fluctuations are shown to agree with the theoretical predictions for both cylindrical and toroidal systems.

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I. INTRODUCTION

Since the pioneering work of Buneman [1] and Dawson [2] in one dimension, particle simulation of plasmas has been developing continuously as more need is required for the understanding of the nonlinearities and many-body properties associated with plasma dynamics. Nonlinear behavior of various microinstabilities, plasma heating associated with the parametric instabilities and plasma diffusion due to convective cells are some of the examples in which the particle simulation played a decisive role for the understanding of the physical processes involved.

Recently, it has been recognized that the particle simulation method can also be very useful in more applied fields of plasma physics directly aimed at the controlled nuclear fusion research. Some of these examples are the simulations of neoclassical diffusion [3], neutral beam injection processes in a tokamak [4] and the impurity sputtering from the wall [5]. For these calculations, self-consistent electric and magnetic fields are usually ignored and the particle orbits are followed in three dimensions for given electric and magnetic fields. For many cases, Monte-Carlo method is often employed to represent the interactions among particles through the Fokker-Planck collision operator.

Most of the self-consistent simulations have been carried out in an idealized system in reduced dimensions. To avoid the interaction with the boundary, periodic boundary conditions are often employed to simulate an infinite system. Furthermore,

unrealistic mass ratios are used so as to shorten the computing time. While some progress has been made for simulating a plasma with realistic parameters in a bounded, finite length system using large mass ratios [6], possibilities of simulating a full three-dimensional large plasma device have not been pursued much so far .

In this paper, we will explore the possibility of simulating large, three-dimensional cylindrical and toroidal plasmas using a hybrid approach of spatial grid and eigenfunction expansion technique for solving the Maxwell equations and for pushing particles. In Sec. II, the model is introduced for a cylinder and a torus of rectangular cross section. For a toroidal system we have developed a finite size particle model retaining up to the dipole terms and the radial Poisson equation is solved by cubic spline technique. Tests of the models are shown in Sec. III including the measurements of the thermal spectrum. Concluding remarks are given in Sec. IV.

II. MODEL

1. Basic Ideas for the Model

It is well known that, for particle simulation of plasmas, there are two major kernels which are most important and also most time consuming. One of them is to solve the Maxwell Equations for the electric and magnetic fields. The other is to push the particles according to the equation of motion.

When one deals with the one dimensional model where the plasmas are represented by a group of positively and negatively

charged sheets, the solution of Maxwell equations is indeed trivial [1,2,7]. The electrostatic field, for example, is constant everywhere except at the particle location where it jumps by the amount of $4\pi\rho$ across a sheet where ρ is the surface charge density. It is sufficient to count the number of positive and negative sheets for determining the electrostatic field.

When a sheet crosses the other sheet during the course of its motion, the electric field on the sheet changes suddenly giving rise to the short range collisional effects as opposed to collective effects due to the ordered motion of many particles. It is well known that the collisional effects in one dimension are small and can be neglected ordinarily [8].

For two-dimensional simulations, the simple picture for fields in one dimensional plasma no longer holds. The electrostatic field, for example, generated by a two dimensional charged rod varies as $1/r$ where r is the distance from the charge and the observer. This field is no longer constant in space and changes its magnitude with r . Furthermore, in contrast to one dimension, it becomes very large and varies very rapidly when two particles come close enough with each other. In other words, the two dimensional collisional effects are overwhelmingly large so that it can wipe out the collective effects easily as was seen in some of the initial effort for the two-dimensional simulations.

The great success of the use of finite-size particles lies on the fact that one can disregard the short range force in a most natural way by assuming a particle has finite size

comparable to the Debye length, thus eliminating the short range, two-body interactions and smoothing out the enhanced collisional effects due to the coarse graininess of the model. Further smoothing is carried out when the force on an extended particle is calculated by using a spatial grid. Here, instead of calculating the exact force on a particle, an approximate force is calculated using the electric and magnetic fields defined on the spatial grid points [9]. It was found that this procedure is equivalent to the multipole expansion in electrodynamics [10]. There is hardly any doubt that the finite size particle model combined with the use of a spatial grid has been the most successful model in particle simulation.

There are also several examples, where the same technique is extended successfully to full three-dimensions using a three dimensional spatial grid [11]. While this model is very efficient in calculating the electric and magnetic fields and the force on a particle, one cannot simulate a large volume of plasma due to the limited capacity of the available computers. Due to the grid instabilities [12,13] the Debye length should not be smaller than a fraction of grid size Δ , say, one half of Δ . Let us assume, for example, one can simulate a system of $64 \times 64 \times 64$ grid using a presently available large scientific computer. Assuming an optimum size of grid, say $\Delta = 2\lambda_D$, the physical size of the system would then be $128 \times 128 \times 128$ Debye cube. Let us compare the size of this simulation with the size of existing real plasma devices. A Q-machine [14]

which is typically used for basic plasma research, has a plasma dimension of $1 \sim 2$ cm radius by $50 \sim 100$ cm long. This would imply a plasma to be a size of $100 \sim 200$ Debye length across by 5×10^4 Debye length long. Therefore, the simulation plasma is large enough for the cross section while it is much too short in the axial direction. Similar conclusions can be drawn for larger fusion devices such as tokamaks or stellarators where the length in the toroidal direction is much longer than the cross-sectional length. This simply indicates that it is not possible to simulate real devices using a most advanced scientific computer to date. Needless to say, one would like to keep the grid quantities such as electric and magnetic fields in the central core of a computer while keeping the particle data in the outside device such as disks. Because of the fact that the grid quantities are randomly accessed, transferring the large grid in and out between disks and main cores would be painfully time consuming and we should consider some other way to save the situation.

While the axial length of the real devices is much longer than the dimension of a cross section, we know theoretically and by laboratory experiments that most of the important physics for plasma confinement are associated with the modes of very long wavelength along the field lines compared with the perpendicular wavelength ($k_{\perp} \gg k_{\parallel}$). Such examples are low frequency drift instabilities, trapped particle instabilities, lower hybrid waves and the hydromagnetic instabilities including kink, tearing and Alfvén modes. This fact suggests that when simulating

these phenomena, one need not keep very many grid points in the axial direction. In fact, the variation along the field lines is very slow compared with that in the cross section and therefore keeping only the reasonable number of the long wavelength modes in the axial direction should be sufficient. This naturally suggests a new type of simulation model using a normal mode expansion in place of a spatial grid in the axial direction while using the standard grid expansion in a two dimensional cross section. As will be shown, this model is quite useful for simulating realistic plasmas using presently available computers. It may be necessary, depending on the problems investigated, to build in a collision operator through the Monte-Carlo technique for random process. This will partially compensate for the neglect of the short wavelength fluctuations which are responsible for the collisional effects.

2. Cylindrical Model

Let us consider, as the first example, a three-dimensional slab model of a rectangular cross section shown in Fig. 1. A toroidal model is considered later. Assume a particle has finite size given by the Gaussian charge density [10]

$$\rho_j(x,y,z) = \frac{q_j}{(2\pi)^{3/2} a_x a_y a_z} \exp \left[- \left(\frac{(x-x_j)^2}{2a_x^2} + \frac{(y-y_j)^2}{2a_y^2} + \frac{(z-z_j)^2}{2a_z^2} \right) \right] \quad (1)$$

where (x_j, y_j, z_j) is the location of the center of the j -th particle, q_j is its total charge and a_x , a_y and a_z are the particle size in three directions. We consider an electrostatic field only in this paper although the extension to include the fully electromagnetic or magnetostatic interactions is straightforward.

The Poisson equation for the electrostatic field would then be

$$\nabla^2 \phi = -4\pi \sum_j \frac{q_j}{(2\pi)^{3/2} a_x a_y a_z} \exp \left[- \left(\frac{(x-x_j)^2}{2a_x^2} + \frac{(y-y_j)^2}{2a_y^2} + \frac{(z-z_j)^2}{2a_z^2} \right) \right] \quad (2)$$

We will avoid the numerical difficulties arising from the use of cylindrical coordinate throughout the paper, since we believe the Cartesian coordinate is much more superior to the cylindrical one in many aspects for numerical computations.

As described in the previous section, let us expand ϕ in terms of eigenfunctions which are simply $\exp(ik_z z)$ for the slab model where $k_z = 2\pi n/L_z$. L_z is the length of the system which is assumed periodic in z .

$$\phi(x, y, z) = \sum_{n=-N}^N \phi_n(x, y) \exp \left(i \frac{2\pi n z}{L_z} \right) \quad (3)$$

where N is the number of modes in z one would like to keep in the model.

Similarly the charge density $\rho(x,y,z)$ is expanded in the same manner,

$$\rho(x,y,z) = \sum_{n=-N}^N \rho_n(x,y) \exp\left(i \frac{2\pi n z}{L_z}\right) \quad (4)$$

where

$$\begin{aligned} \rho_n(x,y) &= \frac{1}{L_z} \int_0^{L_z} \rho(x,y,z) \exp\left(-i \frac{2\pi n z}{L_z}\right) dz \\ &= \frac{1}{2\pi a_x a_y L_z} \exp\left(-\frac{k_z^2 a_z^2}{2}\right) \sum_j \exp\left[-\left(\frac{(x-x_j)^2}{2a_x^2} + \frac{(y-y_j)^2}{2a_y^2}\right)\right] \\ &\quad \exp(-ik_z z_j) \end{aligned} \quad (5)$$

The equation for $\phi_n(x,y)$ is then found from (2), (3), (4) and (5).

$$\left[\nabla_{xy}^2 - \left(\frac{2\pi n}{L_z}\right)^2\right] \phi_n(x,y) = -4\pi \rho_n(x,y) \quad (6)$$

Equation (6) is basically the Poisson equation in two-dimensions which can be solved by means of multipole expansion scheme around the nearest grid point using the fast Fourier transform (FFT)[10].

Let us outline, for the sake of completeness, the multipole expansion method briefly here.

Let us first Fourier transform Eq. (6) with respect to x and y coordinates. Assuming a periodic boundary conditions in both x and y , we find

$$-\left[\left(k_x^2 + k_y^2\right) + \left(2\pi n/L_z\right)^2\right] \bar{\phi}_n(k_x, k_y) = -4\pi \bar{\rho}_n(k_x, k_y)$$

where

$$\begin{aligned} \bar{\rho}_n(k_x, k_y) &= \frac{1}{L_x L_y} \int_0^{L_x} x \int_0^{L_y} y \rho_n(x, y) \exp\left[-i(k_x x + k_y y)\right] dx dy \\ &= \frac{1}{L_x L_y L_z} \exp\left[-\left(k_x^2 a_x^2 + k_y^2 a_y^2 + k_z^2 a_z^2\right)/2\right] \sum_j \exp\left[-i\left(k_z z_j + \right.\right. \\ &\quad \left.\left. k_x x_j + k_y y_j\right)\right] \end{aligned}$$

Here $k_x = 2\pi\ell/L_x$ and $k_y = 2\pi m/L_y$.

Introducing a two dimensional spatial grid in the x - y plane, we expand (x_j, y_j) around its nearest grid point, i.e., $x_j = n_j^x \Delta + \delta x_j$, $y_j = n_j^y \Delta + \delta y_j$ where (n_j^x, n_j^y) is the nearest grid point of the j -th particle and $(\delta x_j, \delta y_j)$ are the displacements from the nearest grid point.

According to the multipole expansion method, we expand

$\exp(-ik_x x_j) = \exp(-ik_x n_j^x \Delta) (1 - ik_x \delta x_j)$ and $\exp(-ik_y y_j) = \exp(-ik_y n_j^y \Delta) (1 - ik_y \delta y_j)$ keeping up to the dipole moments for each particle. We will keep the $e^{-ik_z z_j}$ term unexpanded here because there is no grid in the z direction. Then $\bar{\rho}_n(k_x, k_y)$ would then be

$$\bar{\rho}_n(k_x, k_y, k_z) = \frac{1}{L_x L_y L_z} \exp\left[-\left(k_x^2 a_x^2 + k_y^2 a_y^2 + k_z^2 a_z^2\right)/2\right] \sum_{s=1}^{L_x} \sum_{s'=1}^{L_y} \left(\rho_{ss'}, -ik_x \delta\rho_{ss'}^x, -ik_y \delta\rho_{ss'}^y\right) \exp\left[-i2\pi\left(\frac{s\ell}{L_x} + \frac{s'm}{L_y}\right)\right] \quad (8)$$

where $\rho_{ss'}$, and $\delta\rho_{ss'}^x$, $\delta\rho_{ss'}^y$, are the monopole and the dipole charge densities at the (s, s') grid point weighted by the eigenfunction $e^{-ik_z z_j}$. They are defined by

$$\rho_{ss'} = \sum_j q_j \exp(-ik_z z_j) U(s\Delta - x_j) U(s'\Delta - y_j),$$

$$\delta\rho_{ss'}^x = \sum_j q_j \exp(-ik_z z_j) (x_j - s\Delta) U(s\Delta - x_j) U(s'\Delta - y_j)$$

and

$$\delta\rho_{ss'}^y = \sum_j q_j \exp(-ik_z z_j) (y_j - s'\Delta) U(s\Delta - x_j) U(s'\Delta - y_j)$$

where

$$U(x-x_j) = \begin{cases} 1 & \text{for } |x - x_j| < \Delta/2 \\ 0 & \text{for } |x - x_j| > \Delta/2 \end{cases}$$

and the summation j is over all the particles. Here L_x and L_y are the length of the system in x and y in terms of the grid size Δ and therefore they correspond to the total number of grid points in each direction. It is clear that the double summation of the RHS of Eq. (8) is the two dimensional FFT of the weighted monopole and dipole charge densities on the grid points. It is straightforward to find the potential $\phi_n(x,y)$ by the inverse fast Fourier transform of $\phi_n(k_x, k_y)$ with respect to (k_x, k_y) , i.e.,

$$\phi_n(s\Delta, s'\Delta) = \sum_{\ell=1}^{L_x} \sum_{\ell'=1}^{L_y} \phi_n(k_x, k_y) \exp \left[i2\pi \left(\frac{s\ell}{L_x} + \frac{s'\ell'}{L_y} \right) \right]$$

Finally the total potential will be given by summing over n as given by Eq. (3).

It is clear that the simulation method described above takes the full advantage of both multipole expansion method in terms of finite-size particles combined with the FFT technique on a spatial grid and the eigenfunction expansion method in the axial direction which is much longer than the transverse dimension and would be too long to be represented in terms of a spatial grid.

Let us now calculate the force on a finite-size particle which is necessary in the equation of motion [10]. The electric

field force on the j -th particle will be given by

$$\begin{aligned} \tilde{F}(x_j, y_j, z_j) = q_j \int \tilde{E}(x, y, z) \frac{1}{(2\pi)^{3/2} a_x a_y a_z} \\ \exp \left[- \left(\frac{(x-x_j)^2}{2a_x^2} + \frac{(y-y_j)^2}{2a_y^2} + \frac{(z-z_j)^2}{2a_z^2} \right) \right] dx dy dz \end{aligned} \quad (9)$$

where $\tilde{E}$ is calculated from ϕ and is assumed to take the form of

$$\tilde{E}(x, y, z) = \sum_{n=-N}^N \tilde{E}_n(x, y) \exp \left(\frac{-2\pi i n z}{L_z} \right)$$

The z integration can be carried out to find for the force in the x -direction

$$\begin{aligned} F_x(x_j, y_j, z_j) = \frac{q_j}{2\pi a_x a_y} \sum_{n=-N}^N \exp \left(\frac{-k_z^2 a_z^2}{2} \right) \exp(i k_z z_j) \iint \tilde{E}_{nx}(x, y) \\ \exp \left[- \left(\frac{(x-x_j)^2}{2a_x^2} + \frac{(y-y_j)^2}{2a_y^2} \right) \right] dx dy \end{aligned}$$

According to the procedure of multipole expansion scheme [10], F_x is now Fourier transformed with respect to x_j and y_j . Then

$$\begin{aligned} F_x(k_x, k_y, k_z) = q_j \sum_{n=-N}^N \exp \left(\frac{-k_z^2 a_z^2}{2} \right) \exp(i k_z z_j) \tilde{E}_{nx}(k_x, k_y) \\ \exp[-(k_x^2 a_x^2 + k_y^2 a_y^2)/2] \end{aligned} \quad (10)$$

$F_x(x_j, y_j, z_j)$ is calculated from the inverse FFT of (10) and is expanded at around the nearest grid point, that is,

$$F_x(x_j, y_j, z_j) = F_x(n_j^x \Delta, n_j^y \Delta, z_j) + \delta x_j \frac{\partial F_x}{\partial x} + \delta y_j \frac{\partial F_x}{\partial y}$$

keeping up to the dipole terms. The derivatives of F_x are evaluated at the nearest grid point and are calculated by differencing F_x 's on the neighboring points.

In the actual simulations, ions are pushed using the full Lorentz force while the electrons are assumed being guiding center particles. The standard predictor-corrector scheme is used for the electron orbit integration to keep the higher order of accuracy [6]. As will be shown in Sec. III, the model works successfully to produce the expected thermal spectrum.

3. Toroidal Model

After studying the new model for the cylindrical system, let us now consider a toroidal application. Consider a torus of rectangular cross section as shown in Fig. 2. The Poisson equation in this coordinate takes the form of

$$\frac{\partial^2 \Phi}{\partial r^2} + \frac{1}{r} \frac{\partial \Phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\partial^2 \Phi}{\partial z^2} = -4\pi \rho(r, \phi, z) \quad (11)$$

where $\Phi(r, \phi, z)$ is the electrostatic potential and is usually assumed to vanish on the surrounding conducting wall. We will solve this equation by expanding the potential and charge density in terms of the eigenfunction in ϕ and the multipole expansion

around the nearest grid point on the rectangular grid introduced in the poloidal cross section as before.

Now expanding Φ and ρ in the toroidal direction,

$$\begin{aligned}\Phi(r, \phi, z) &= \sum_{n=-N}^N \Phi_n(r, z) \exp(in\phi) \\ \rho(r, \phi, z) &= \sum_{n=-N}^N \rho_n(r, z) \exp(in\phi)\end{aligned}$$

Eq. (11) is reduced to

$$\frac{\partial^2 \Phi_n}{\partial r^2} + \frac{1}{r} \frac{\partial \Phi_n}{\partial r} - \frac{n^2}{r^2} \Phi_n + \frac{\partial^2 \Phi_n}{\partial z^2} = -4\pi \rho_n \quad (12)$$

which is to be solved on a two-dimensional grid.

To see how the multipole expansion method works for the toroidal system, let us Fourier transform the charge density with respect to ϕ first.

$$\begin{aligned}\rho_n(r, z) &= \frac{1}{2\pi} \int_0^{2\pi} \rho(r, \phi, z) e^{-in\phi} d\phi \\ &= \frac{1}{(2\pi a^2)^{3/2}} \sum_j q_j \exp \left\{ - \left[(z-z_j)^2 + (r-r_j)^2 + 2rr_j \right] / 2a^2 \right\} \\ &\quad \cdot I_n(rr_j/a^2) \exp(in\phi_j) ,\end{aligned}$$

where I_n is the modified Bessel function and the use of the identity

$$\exp(\lambda \cos \phi) = \sum_{n=-\infty}^{\infty} I_n(\lambda) \exp(in\phi)$$

is made. For simplicity, we have assumed that a finite-size particle is isotropic ($a_x = a_y = a_z = a$).

Assuming the particle size a is of the order of the grid size and r and r_j are of the order of the major toroidal radius R_0 , we note the expansion

$$\begin{aligned} \exp(-rr_j/a^2) I_n(rr_j/a^2) &= \frac{1}{(2\pi rr_j/a^2)^{1/2}} [1 + O(\frac{n^2 a^2}{rr_j})] \\ &\approx (2\pi rr_j/a^2)^{-1/2} \\ &\approx (2\pi/a^2)^{-1/2} \frac{1}{r_j} \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right) \end{aligned}$$

gives a good approximation. Thus,

$$\begin{aligned} \rho_n(r, z) &\approx \frac{1}{(2\pi a)^2} \sum_j q_j \exp\left[-\left((z-z_j)^2 + (r-r_j)^2\right)/2a^2\right] \\ &\quad \frac{\exp(-in\phi_j)}{r_j} \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right) \end{aligned} \quad (13)$$

Fourier transforming $\rho_n(r, z)$ with respect to z , we find

$$\begin{aligned}\rho_n(r, k_z) &= \frac{1}{L_z} \int_0^{L_z} \rho_n(r, z) \exp(-ik_z z) dz \\ &= \frac{\exp(-k_z^2 a^2/2)}{(2\pi)^{3/2} a L_z} \sum_j q_j \exp\left[-i(n\phi_j + k_z z_j)\right] \\ &\quad \cdot \exp\left[-(r-r_j)^2/2a^2\right] \frac{1}{r_j} \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right)\end{aligned}$$

We note immediately that the fast Fourier transform may be employed in the z -direction. Writing $z_j = n_j^z \Delta z + \delta z_j$ where n_j^z is the nearest grid point in z for the j -th particle, we find

$$\begin{aligned}\rho_n(r, k_z) &\approx \frac{\exp(-k_z^2 a^2/2)}{(2\pi)^{3/2} a L_z} \sum_j q_j \exp\left[-i(n\phi_j + k_z n_j^z \Delta z)\right] (1 - ik_z \delta z_j) \\ &\quad \exp\left[-(r-r_j)^2/2a^2\right] \frac{1}{r_j} \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right)\end{aligned} \tag{14}$$

Finally we note in the r direction, the fast Fourier transform may not be appropriate since the system, Eq. (12), is aperiodic in the radial direction and obviously the trigonometric functions are not the eigenfunctions. Therefore, instead of using the fast Fourier transforms, we solve Eq. (12) by means of a spline method as described later. However, to determine the charge

density on the radial grid in terms of multipole expansion method, we will use the fast Fourier transform. Since the charge density and the potential vanish at the boundaries at $r = R_1$ and R_2 , we will consider the systems periodic by including its antisymmetric parts.

Fourier transforming $\rho_n(r, k_z)$ with respect to r , we find

$$\begin{aligned} \bar{\rho}_n(k_r, k_z) &= \frac{1}{L_R} \int_0^{L_R} \rho_n(R_1+s, k_z) \exp(-ik_r s) ds \\ &\equiv \frac{\exp(-k_z^2 a^2/2)}{2\pi L_R L_z} \sum_j q_j \exp\left[-i\left(n\phi_j + k_z n_j^z \Delta z\right)\right] (1 - ik_z \delta z_j) \\ &\quad \cdot \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} \exp\left[-(r-r_j)^2/2a^2 - ik_r(r-R_1)\right] \\ &\quad \cdot \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right) \frac{d(r-r_j)}{r_j} \end{aligned} \quad (15)$$

The r integral may be carried out easily to find

$$\begin{aligned} I_{kr} &\equiv \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} \frac{\exp[-(r-r_j)^2/2a^2]}{r_j} \left(1 - \frac{1}{2} \frac{r-r_j}{r_j}\right) \exp[-ik_r(r-R_1)] d(r-r_j) \\ &= \frac{\exp[(-k_r^2 a^2)/2]}{r_j} \left(1 - \frac{1}{2i} \frac{k_r a^2}{r_j}\right) \exp[-ik_r(r_j - R_1)] \end{aligned}$$

Introducing a radial grid with the uniform width Δr , $r_j = R_1 + n_j^r \Delta r + \delta r_j$ and keeping only up to the dipole term, I_{kr} becomes

$$I_{kr} = \frac{\exp(-k_r^2 a^2/2)}{r_j} \left(1 - \frac{1}{2i} \frac{k_r a^2}{r_j}\right) \exp(-ik_r n_j^r \Delta r) (1 - ik_r \delta r_j) \quad (16)$$

We note that the toroidal effect on the finite size particle is $O(k_r a^2/r_j)$ which is quite small for $k_r a \lesssim 1$. Then $\bar{\rho}_n(k_r, k_z)$ becomes

$$\begin{aligned} \bar{\rho}_n(k_r, k_z) = & \left(1 - \frac{1}{2i} \frac{k_r a^2}{R_0}\right) \frac{\exp[-(k_z^2 + k_r^2) a^2/2]}{L_R L_z 2\pi} \sum_{s=1}^{L_z} \sum_{s'=1}^{L_R} \\ & \frac{(\rho_{ss'} - ik_r \delta \rho_{ss'}^r - ik_z \delta \rho_{ss'}^z)}{r_{s'}} \exp(-i2\pi s \ell / L_z) \\ & \cdot \exp(-i2\pi s' \ell' / L_R) \end{aligned} \quad (17)$$

where $k_z = 2\pi \ell / L_z$, $k_r = 2\pi \ell' / L_R$, and $\rho_{ss'}$ and $\delta \rho_{ss'}^{z,r}$ are the nearest grid point and the dipole charge contributions at the grid point (s, s') weighted by the $e^{-in\phi_j}$ defined by

$$\rho_{ss'} = \sum_j q_j e^{-in\phi_j} U(s\Delta z - z_j) U(R_1 + s'\Delta r - r_j) ,$$

$$\delta\rho_{ss'}^z = \sum_j q_j e^{-in\phi_j} (z_j - s\Delta z) U(s\Delta z - z_j) U(R_1 + s'\Delta r - r_j)$$

and

$$\delta\rho_{ss'}^r = \sum_j q_j e^{-in\phi_j} (r_j - R_1 - s'\Delta r) U(s\Delta z - z_j) U(R_1 + s'\Delta r - r_j)$$

In Eq. (17) the expansion of the finite size particles up to the dipole moment about the nearest grid point has been carried out both in z and r directions using a $(r-z)$ rectangular mesh while in the toroidal direction, no expansion is made and the eigenfunction $e^{-in\phi}$ is used all the way keeping the reasonable number of modes in that direction.

Inverting the finite Fourier transform of $\bar{\rho}_n(k_r, k_z)$, with respect to k_r , we obtain the charge density on the radial grid points $\rho_n(R_1 + n^r\Delta r, k_z)$. The Poisson equation in r direction finally becomes

$$\left[\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \left(\frac{n^2}{r^2} + k_z^2 \right) \right] \phi_n(r, k_z) = -4\pi\rho_n(r, k_z) \quad (18)$$

where $\rho_n(r, k_z)$ is calculated by inverting Eq. (17) numerically. The radial equation (18) has been solved by using the cubic spline technique as described below [15,16]. Cubic spline has been applied successfully in integrating the nonlinear Vlasov equation [16].

Let $f_i (i = 1, \dots, N)$ be the values of a function f on N equally spaced grid points with a width Δ . Using cubic splines

we write for the interpolation functions

$$y_i(r) = f_i + P_i \frac{(r-r_i)}{\Delta} + \frac{1}{2} S_i \frac{(r-r_i)^2}{\Delta^2} + g_i \frac{(r-r_i)^3}{\Delta^3} \quad (19)$$

where $r_{i-1} \leq r \leq r_{i+1}$. From the condition that the function and its derivatives are continuous at the grid points, it is easy to show that the recurrence formula for P_i 's and S_i 's are

$$3(f_i - f_{i+1}) + P_{i+1} + 2P_i + \frac{1}{2}S_i = 0 \quad (20)$$

and

$$P_{i-1} + 4P_i + P_{i+1} = 3(f_{i+1} - f_{i-1}) \quad (21)$$

where $\Delta = 1$ is assumed. From Eq. (19) we immediately see that P_i and S_i correspond to the values of $dy_i/dr|_{r=r_i}$ and $d^2y_i/dr^2|_{r=r_i}$ respectively. If we write the radial Poisson equation (18) in a finite difference form and approximate the first and second derivatives of the potential by the spline values, Eq. (18) becomes

$$S_i + B_i P_i + C_i f_i = \rho_i \quad (22)$$

where B_i, C_i are constant coefficients associated with Eq. (18) and ρ_i stands for the density on the radial mesh. Now eliminating S_i and P_i from Eqs. (20), (21), and (22), we arrive at the final difference equation

$$\begin{aligned}
 & \left\{ \frac{(B_i - 4) [2(C_{i-1} - 6(B_{i-1} - 4))] }{4 + (B_{i-1} - 4)(B_i + 4)} \right\} f_{i-1} \\
 & + \left\{ (C_i - 6) + \frac{(B_i - 4) [12 - (B_{i-1} - 4)(C_i - 6)] }{[4 + (B_{i-1} - 4)(B_i + 4)]} + \frac{2[6(B_i - 4) - 2(C_i - 6)] }{4 + (B_i - 4)(B_{i+1} + 4)} \right\} f_i \\
 & + \left\{ 6 - \frac{2[12 - (B_i - 4)(C_{i+1} - 6)] }{4 + (B_i - 4)(B_{i+1} + 4)} \right\} f_{i+1} = \left[\frac{2(B_i - 4)}{4 + (B_{i-1} - 4)(B_i + 4)} \right] \rho_{i-1} \\
 & + \left[1 - \frac{(B_{i-1} - 4)(B_i - 4)}{4 + (B_{i-1} - 4)(B_i + 4)} - \frac{4}{4 + (B_i - 4)(B_{i+1} + 4)} \right] \rho_i \\
 & + \left[\frac{2(B_i - 4)}{4 + (B_i - 4)(B_{i+1} + 4)} \right] \rho_{i+1} \tag{23}
 \end{aligned}$$

This equation can be solved with appropriate boundary conditions. The error analysis of spline has been given in many places [15] and is proportional to Δ^4 . The above scheme has been tested for solving the Poisson equation where the solution is known analytically to be a Bessel function. The numerical results are found to agree with the analytic results within the sufficient accuracy.

Now let us briefly calculate the force on a finite size particle. The electric force for a particle at (r_j, ϕ_j, z_j) is given by

$$\tilde{F}(r_j, \phi_j, z_j) = q_j \int \tilde{E}(r, \phi, z) \frac{1}{(2\pi a^2)^{3/2}} \exp \left\{ - \left[(z-z_j)^2 + r^2 + r_j^2 \right] / 2a^2 \right\} \\ \exp \left[\frac{rr_j}{a^2} \cos(\phi - \phi_j) \right] r dr d\phi dz$$

where $\tilde{E}(r, \phi, z)$ is calculated from $\phi_n(k_r, k_z)$ and is given by, for example,

$$E_z(r, \phi, z) = \sum_{n=-N}^N E_n(r, z) \exp(in\phi)$$

Then

$$F_z(r_j, \phi_j, z_j) = \sum_{n=-N}^N q_j \frac{\exp(in\phi_j)}{(2\pi)^{1/2} a^3} \int E_{nz}(r, z) \exp \left\{ - \left[(z-z_j)^2 + r^2 + r_j^2 \right] / 2a^2 \right\} \\ \cdot I_n \left(\frac{rr_j}{a^2} \right) r dr dz \\ \approx \sum_{n=-N}^N q_j \frac{\exp(in\phi_j)}{2\pi a^2} \int E_{nz}(r, z) \exp \left\{ - \frac{\left[(z-z_j)^2 + (r-r_j)^2 \right]}{2a^2} \right\} \\ \cdot \left(1 + \frac{r-r_j}{2r_j} \right) dr dz$$

Now following the procedure of multipole expansion scheme, let us Fourier transform the force $F_z(r_j, \phi_j, z_j)$ with respect to (r_j, z_j)

$$F_z(k_r, \phi_j, k_z) = \sum_{n=-N}^N \frac{q_j \exp(in\phi_j)}{2\pi a^2} \int dr dz \int_{R_1}^{R_2} dr_j \int_0^{L_z} dz_j$$

$$\cdot \exp\left\{-\left[(z-z_j)^2 + (r-r_j)^2\right]/2a^2\right\} \left(1 + \frac{r-r_j}{2r_j}\right)$$

$$\cdot \exp\left\{-i\left[k_z z_j + k_r (r_j - R_1)\right]\right\} E_{nz}(r, z)$$

The integral with respect to z and z_j is straightforward to find

$$F_z(k_r, \phi_j, k_z) = \frac{\exp(-k_z^2 a^2/2)}{(2\pi)^{1/2} a} \sum_{n=-N}^N q_j \exp(in\phi_j) \int dr \int_{R_1}^{R_2} dr_j E_{nz}(r, k_z)$$

$$\cdot \exp\left[-(r-r_j)^2/2a^2\right] \left(1 + \frac{r-r_j}{2r_j}\right) \exp\left[-ik_r (r_j - R_1)\right]$$

The integral over r and r_j is also carried out by approximating

$(r-r_j)/2r_j \cong (r-r_j)/2R_0$. Then

$$F_z(k_r, \phi_j, k_z) = \exp\left[-(k_z^2 a^2 + k_r^2 a^2)/2\right] \left(1 - \frac{k_r a^2}{2iR_0}\right) \sum_{n=-N}^N q_j \exp(in\phi_j)$$

$$E_{nz}(k_r, k_z) \quad (24)$$

The force on the j -th particle is calculated from the inverse transforms of (24) and then expanded around the nearest grid point. Writing $r_j = n_j^r \Delta r + \delta r_j$ and $z_j = n_j^z \Delta z + \delta z_j$,

$$F_z(r_j, \phi_j, z_j) = F_z(n_j^r \Delta r, \phi_j, n_j^z \Delta z) + \delta r_j \frac{\partial F_z}{\partial r} + \delta z_j \frac{\partial F_z}{\partial z}$$

where the derivatives of F_z are evaluated at the nearest grid point and are calculated by differencing F_z 's on the neighboring points.

The evolution of the system is obtained by pushing ions with the full Lorentz force and integrating the guiding center drift equations for electrons. The electron guiding center equations are given by

$$\frac{d\tilde{r}}{dt} = \frac{(\tilde{v} \cdot \tilde{B})}{B^2} \tilde{B} + \frac{c \tilde{E} \times \tilde{B}}{B^2} - \frac{1}{\Omega_e B^2} \left(\frac{\mu B}{m_e} + v_{||}^2 \right) \tilde{B} \times \nabla \tilde{B}$$

$$\frac{dv_{||}}{dt} = - \frac{q}{m_e} \frac{\mathbf{E} \cdot \mathbf{B}}{B} - \frac{1}{m_e B} \nabla (\mu B) + \frac{c v_{||}}{B^3} (\mathbf{E} \cdot \mathbf{B}) \cdot \nabla B$$

$$\mu = \frac{m v_{\perp}^2}{2B} = \text{constant} \quad (25)$$

where $v_{||} = \frac{\mathbf{v} \cdot \mathbf{B}}{B}$ and $\Omega_e = \frac{eB}{m_e c}$.

The integration scheme used is a second order predictor-corrector scheme known as modified Euler method [17]. Symbolically the guiding center equation can be written as $d\mathbf{r}/dt = \mathbf{v}(\mathbf{r}, t)$. Then the time difference scheme is

$$\begin{aligned} \bar{\mathbf{r}}_{n+1} &= \mathbf{r}_{n-1} + 2\Delta t \mathbf{v}(\mathbf{r}_n, t_n) \\ \mathbf{r}_{n+1} &= \mathbf{r}_n + \frac{\Delta t}{2} \left[\mathbf{v}(\mathbf{r}_n, t_n) + \mathbf{v}(\bar{\mathbf{r}}_{n+1}, t_{n+1}) \right] \end{aligned} \quad (26)$$

Note that this scheme requires two solutions of the Poisson equation per time step.

III. TEST OF THE MODEL

After developing the cylindrical and toroidal models described above, we have tested the codes by measuring the total energy conservation, thermal fluctuation spectrum and the particle orbit.

1. Test of the Cylindrical Model

Let us briefly describe the test results from the three-dimensional slab model. We consider a simple system in which the magnetic field is uniform and in the z-direction only. The plasma is assumed uniform and is periodic in y- and z-directions while it is bounded between $x = 0$ and L_x due to the conducting walls which reflect particles in the same manner described in Ref. 6.

Figure 3 shows the time averaged thermal spectrum for different modes of $\mathbf{k} = (k_x, k_y, k_z) = (2\pi m/L_x, 2\pi n/L_y, 2\pi \ell/L_z)$ where the size of the box was chosen $(L_x, L_y, L_z) = (32, 32, 32)$. In this particular example, 9 modes ($\ell = 0, \pm 1, \pm 2, \pm 3, \pm 4$) in z-direction while 32×32 spatial mesh was employed in the x-y plane. The other parameters of simulations are 2^{12} particles for ions and electrons respectively, $\Omega_e/\omega_{pe} = 5$, $T_e = T_i$, $m_i/m_e = 25$, $v_e = 2$, $a = \Delta = 1$ and $\omega_{pe} \Delta t = 1$. Ω_e is the electron gyrofrequency, v_e is the electron thermal speed, a is the Gaussian particle size which is taken isotropic in three directions, and Δt is the time integration step size. We note that the fluctuation spectrum averaged over $\omega_{pe} t = 0 \sim 50$ is in good agreement with the theoretical prediction

$$\frac{E_k^2}{8\pi} = \frac{T}{2} \frac{1}{1 + k^2 \lambda_D^2 \exp(k^2 a^2)}$$

as shown by the solid line. The total energy conservation was about 0.5% at the end of the calculation. This may be due to, for example, too large time step of integration or too few particles per Debye sphere. Electrons were pushed by the guiding center drift equation in the transverse direction while the electron parallel motion was followed exactly. Ions were pushed exactly. Full dipole calculations were employed in this example which took about 10 seconds for one iteration for 2^{13} particles on the IBM 360/91 for a Fortran code. NGP calculations are expected to be much faster which may be required for large, three-dimensional calculations to be finished within a reasonable computing time.

We have simulated the same example shown above with the number of modes in z doubled ($\ell = 0, \pm 1, \pm 2, \dots, \pm 9$). It is observed that the shorter wavelength modes also satisfy the energy partition law as well. There were no significant differences observed for the gross behavior of plasmas such as total energy conservation for both cases. This is an encouraging observation since it indicates that we need not keep many modes in the axial direction. When the length of the system is longer compared with the transverse dimension, it may be useful to use anisotropic Gaussian particles elongated in the axial direction.

2. Test of the Toroidal Model

In the toroidal model the imposed magnetic field is taken to be $\vec{B} = \hat{e}_\theta B_\theta + \hat{e}_\phi B_\phi$, where

$$B_\phi(r) = B_\phi^{(0)} R_O / r$$

$$B_\theta = \bar{r} B_\phi^{(0)} / q(\bar{r}) R_O = \frac{\bar{r} B_\phi^{(0)}}{q^{(0)} R_O} \left(1 - \frac{\bar{r}^2}{2\bar{a}^2} \right)$$

and

$$r = R_O + \bar{r} \cos \theta$$

The coordinate $(\bar{r}, \theta)$ measures the position in the cross-sectional plane of the torus with $\bar{r}$ the distance from the minor axis and θ measured from the toroidal plane to the inside. R_O and $\bar{a}$ are the major and minor radius respectively, and $q^{(0)}$ is the safety factor and $B_\phi^{(0)}$ the toroidal field at the minor radius. The plasma is assumed to be bounded due to the conducting walls which reflect particles.

Initially the plasma density and temperature profiles are taken to be Gaussians with, e.g.,

$$n(\bar{r}) = \frac{2 e^{-\bar{r}^2 / C \bar{a}^2}}{C \bar{a}^2 (1 - e^{-1/C})}$$

The constant C characterizes the degree of nonuniformity. The plasma is locally Maxwellian. Fig. 4 shows the fluctuation spectrum averaged over the r -direction for different modes

of

$$(k_z, k_\phi) = \left(\frac{2\pi\ell}{L_z}, \frac{n}{R_o} \right).$$

The size of the torus is taken $\bar{a} = 16$, $R_o = 40$. There are nine modes ($n = 0, \pm 1, \pm 2, \pm 3, \pm 4$) in the toroidal direction ϕ and 32×32 spatial mesh was employed in the r - z cross-sectional plane. The other parameters of the run are 2^{12} particles for each species, $\Omega_e/\omega_{pe} = 4$, $T_e/T_i = 10$, $m_i/m_e = 100$, $\lambda_{De} = 2$, a (particle size) = 1 and $\omega_{pe} \Delta t = 1$, $C_{Ti} = C_{Te} = 0.25$, $C_{ni} = C_{ne} = 0.5$, where Ω_e is the electron gyrofrequency at the minor radius, ω_{pe} is the average electron plasma frequency, C_T and C_n denote temperature and density nonuniformity and $T_e/T_i = 10$ at the minor radius.

As we can see, the agreement between the theoretical predictions and the numerical results averaged over $\omega_{pe} t = 50 \sim 100$ is quite satisfactory. The theoretical fluctuation spectrum averaged over the radial direction for a finite size particle system is given by

$$\int r dr \frac{|E(r, n, \ell)|^2}{8\pi} / \left(\frac{T}{2L_R} \right) = \frac{1}{2\pi\lambda_D} \int_0^{\pi\lambda_D} \frac{dx}{1 + (y^2 + x^2) \exp[(y^2 + x^2)a^2/\lambda_D^2]}$$

where $y^2 = (n^2/R_o^2 + \ell^2 \Delta k_z^2) \lambda_D^2$ and is shown by the solid line. The error for the total energy conservation at the end of the calculation ($\omega_{pe} t = 100$) is about 4%. This may be due to too large time step of integration, too few particles per Debye sphere, the reflecting boundary walls which exert external force on the particles.

Full dipole expansion was employed in this example which took about 15 seconds for one time step for 2^{13} particles on the IBM 360/91 for an unoptimized Fortran code.

IV. Concluding Remarks

We have developed a new class of three dimensional simulation models for cylindrical and toroidal geometry by employing a hybrid approach of eigenfunction expansion and the multipole expansion on a spatial grid. The model is particularly useful for a system in which the axial length is much longer than the transverse dimension as seen for most of the experimental device for controlled fusion such as a tokamak, stellarator and a z-pinch.

Preliminary results for the test of the models are quite satisfactory and are encouraging for the application to more realistic problems. Full three dimensional simulations for the drift wave and trapped particle instabilities are now studied by extending the previous slab model [6,18].

The other important area in which the model described may be very useful is the low frequency hydromagnetic behavior of a plasma in cylindrical and toroidal systems from the microscopic point of view. In particular, kink-tearing modes may be conveniently simulated by keeping several modes in the toroidal direction such as seen for the tokamak experiments. The present model is quite general including most of the kinetic effects in contrast to fluid model so that, for example, the coupling of kink-tearing mode with the other low frequency modes such as drift or Alfvén waves may be seen. It is, of course,

necessary to build in the self-consistent magnetic field in addition to the electrostatic electric field. It may be also necessary to include the short wavelength collisional effects in terms of Monte Carlo method [4] which conveniently compensates the neglect of the short wavelength modes in the toroidal direction. Such a program is in progress and will be reported in the future.

One other remark is ready for the method we developed for the simulation of toroidal plasmas. Because of the finite size of the particles, we calculated the grid charge density by Fourier transforming the exact charge density and then kept it up to the dipole term. Then the grid charge density was transformed back to physical space with respect to radial coordinate since the Poisson equation was solved on the radial mesh points by means of spline technique. This potential had to be transformed to k_r space to calculate the force on a particle up to the dipole term. It is clear that if we could solve the radial Poisson equation in the transformed space rather than the physical mesh points, then two one-dimensional transforms would be saved. One obvious candidate is to make use of the Hankel (Bessel) transform [19] in the radial direction instead of the Fourier transform since the Bessel function is the eigenfunction of the Poisson equation given by (18). We are investigating this alternate method as well and the results will be reported elsewhere.

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Fig. 1. A sketch for the three-dimensional slab model. Spatial grid is used in x-y plane while the mode expansion is employed in z-direction.

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Fig. 2. A sketch for the toroidal model in the rectangular cross section. Note the coordinate chosen in the model.

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Fig. 3. Fluctuation spectrum for the three dimensional slab model described in the test. Time-averaged simulation result agrees well with the theoretical predictions.

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Fig. 4. Fluctuation spectrum averaged over the radial direction for the toroidal model described in the test. Time averaged simulation result agrees well with the theoretical prediction shown by the solid line. The enhancement for long wavelength modes is presumably due to the VB drift which separates the ions from the electrons in the z-directions.