INTRODUCTION TO PARTICLE SIMULATION MODELS AND THEIR APPLICATION TO ELECTROSTATIC PLASMA WAVES IN SPACE

H. Okuda

Plasma Physics Laboratory, Princeton University
Princeton, New Jersey 08544, U.S.A.

ABSTRACT

In the first part of this article, a review of plasma simulation models using finite-size particles is given with an emphasis on the electrostatic models. Physical properties of such simulation models as well as numerical techniques will be studied in some detail. Modification to plasma kinetic theory, collisions and fluctuations, Vlasov-Landau equations will be derived along with an introduction to a spatial grid, charge-foce interpolation and finite-difference schemes.

In the second part of this article, a study of electrostatic ion cyclotron waves driven by a field-aligned current will be studied by numerical simulations. Recent observations of large amplitude electrostatic ion cyclotron waves (eΦ/T_e=1) and ion conics have renewed wide interest in the physics of auroral field lines. We show by numerical simulations that large amplitude ion cyclotron waves can cause an intense ion heating across magnetic field resulting in the formation of ion conics. In addition, two-dimensional simulations of the electrostatic ion cyclotron waves indicate a possibility of energy condensation into a d.c. structure across magnetic field. Such a d.c. structure is associated with large density modulations, n_max/n_min^-1, across magnetic field and may be responsible for the generation of auroral arc elements.
PART I: Introduction to Particle Simulation
Models in Plasma Physics

1. INTRODUCTION

The subject of the first part of this lecture is numerical plasma simulations using particles in which various models are introduced in order to solve nonlinear Vlasov equation. Physical properties of such simulation models and numerical techniques will be studied in some detail. Some applications to space plasma physics are given in the second part. Recent development in high speed, large scale computers and the advancement of our numerical technique have made it possible to simulate an environment which has direct impact on realistic plasma experiments. Numerical simulation is particularly useful when nonlinear effects are important for which only a limited number of analytic methods are available. Furthermore, one often finds, with a help from numerical simulations, that the results obtained by means of numerical simulations are not what analytic theory predicts or what you have guessed beforehand. One is guided therefore, to develop a different analytic model or a new physical interpretation leading to a discovery of new plasma phenomena.

Among many simulation models, emphasis will be placed on the particle simulation models in which a large number of particles are followed in time in their self-consistent and external electromagnetic fields. Knowledge of such particle orbits or characteristics is equivalent to solving the nonlinear Vlasov equation. Solving the Vlasov equation directly is in general much more difficult than particle simulations, particularly in multi-dimensions. Vlasov equation, which has an infinite degree of freedom, represents a dissipationless plasma in which great care must be taken for numerical smoothing. Particle distributions can be distorted to an arbitrary complex degree so that numerical smoothing must be introduced in order to avoid numerical divergence. In particle simulation, such smoothing is done most naturally through particle collisions.

In Sec.2, we shall introduce particle simulation models using finite-size particles. Modification to plasma kinetic theory including dispersion relations to linear oscillations, collisions and fluctuations are given. In Sec.3, numerical methods using finite-size particles in a spatial grid are introduced along with finite-difference method. Several specific models useful for low frequency plasma waves and large plasma volume are also discussed.
2. ELECTROSTATIC PARTICLE SIMULATION MODELS

2.1 Kinetic Equations

We shall briefly review several fundamental kinetic equations for a plasma and point out their relation to particle simulation models. One of the fundamental kinetic equations is the Klimontovich equation for N-particle distribution functions for electrons and ions. Defining the distribution function for s-species

\[ f_s(x, v, t) = \sum_{j \in S} \delta(x - x_j(t)) \delta(v - v_j(t)). \] (1)

the Klimontovich equation states

\[ \frac{df_s}{dt} = \frac{\partial f_s}{\partial t} + v \cdot \frac{\partial f_s}{\partial x} + \frac{q_s}{m_s} (E + \frac{1}{c} \times B) \cdot \frac{\partial f_s}{\partial v} = 0. \] (2)

The electromagnetic fields \( E \) and \( B \) are determined from Maxwell's equations

\[ \nabla \times E = -\frac{1}{c} \frac{\partial B}{\partial t} \] (3)

\[ \nabla \times B = \frac{4\pi}{c} J + \frac{1}{c} \frac{\partial E}{\partial t} \] (4)

\[ \nabla \cdot E = 4\pi \rho \] (5)

\[ \nabla \cdot B = 0 \] (6)

where

\[ J(x, t) = \int dx q_s f_s(x, v, t) \] (7)

and

\[ \rho(x, t) = \int dv q_s f_s(x, v, t). \] (8)

These equations must be supplemented by the initial and boundary conditions for the uniqueness of their solution. Generally speaking, there is no way of solving the Klimontovich equation analytically since, for example, we have no knowledge of the initial conditions for each plasma particle. The Klimontovich equation which is highly singular is not suitable even for numerical computation. On the other hand, the characteristics of the Klimontovich equation in phase space can be followed with relative ease using a high speed computer. The characteristics of the Klimontovich equation is nothing but the trajectory of each particle in phase space and is defined by

\[ \frac{dv_j}{dt} = \frac{q_j}{m_j} \left[ E(x_j) + \frac{1}{c} v_j \times B(x_j) \right] \] (9)
\[ \frac{dX_j}{dt} = V_j \]  \hspace{1cm} (10)

from which the charge and current densities are defined by
\[ \rho_\delta(X, t) = \sum_S q_j \delta(X - X_j(t)) \]  \hspace{1cm} (11)

and
\[ J_\delta(X, t) = \sum q_j V_j \delta(X - X_j(t)). \]  \hspace{1cm} (12)

This way of solving the Klimontovich equation is best suited for numerical simulations by using large, fast digital computers. Differential equations must first be transformed to finite difference equations before they are programmed into a computer. It often takes only a few microsecond to integrate or "push" the equation of motion for one particle for one time step \( \Delta t \). Thus more than a few thousands to a few millions of particles may be used to simulate a plasma within a reasonable computing time using presently available computers. We shall note here that even a million of simulation particles is far too few to represent a real plasma. Each simulation particle must therefore be regarded as representing a large number of real plasma particles. In this sense a simulation particle may be called a superparticle. The consequence of using such a small number of particles is the enhancement of statistical fluctuations and collisional effects both of which tend to mask collective plasma behavior. In addition, \( \delta \)-function representation of charge and current densities given by Eqs. (11) and (12) must be smoothed out in general. We will discuss in detail how such smoothing is done in numerical simulations.

When the Klimontovich equation is averaged over the ensembles of the initial conditions for N-particles, one obtains the Vlasov equation after neglecting the two-body collisions.
\[ \frac{\partial f_S}{\partial t} + v \cdot \frac{\partial f_S}{\partial x} + \frac{q_S}{m_S} (E + \frac{1}{c} v \times B) \cdot \frac{\partial f_S}{\partial v} = 0. \]  \hspace{1cm} (13)

This equation is formally the same to the Klimontovich equation and its numerical solution requires special cares as the distribution functions evolve into fine structures in phase space.

2.2 Finite-size Particle Model

After discussing plasma kinetic equations, we will describe plasma simulation models using finite-size particles in which only the electrostatic Coulomb interactions are retained. Electromagnetic and relativistic simulations are discussed elsewhere in the book. Historically, the first plasma simulation model developed was the one-dimensional sheet model consisting of zero-thickness charged sheets interacting with each other under the influence of electrostatic
Coulomb forces (Buneman 1959, Dawson 1962). While such a sheet model is useful in one-dimension, much of the computing is exhausted in calculating particle crossing which takes place at a distance much shorter than the Debye length. In plasma simulations, we are generally interested in the collective phenomena whose wavelengths are much longer than the Debye length. Furthermore, it is not obvious how to extend the sheet model into two and three dimensions where the Coulomb force between two particles becomes arbitrarily large as the separation of two particles becomes smaller. Since the force changes very rapidly at close encounter, one must use a small time step for preserving acceptable numerical accuracy. Again we note the informations at wavelengths shorter than the Debye length are not necessary. These considerations lead us to the use of finite-size particle models in plasma simulations in the late 1960's (Hockney 1966; Morse and Nielson. 1969; Birdsall and Fuss. 1969; Kruer et al., 1973). Much more information on plasma simulations using particles can be found in Methods in Computational Physics, Vols. 9 (1970) and Vol. 16 (1976). Hockney and Eastwood (1981), Potter (1973) and Birdsall and Langdon (in press).

Let us now consider a simulation model in which singular distributions of charges and potentials are smoothed out without modifying plasma properties at long wavelengths. Singularities in charge and force may be naturally removed by considering particles with finite extent, instead of classical zero-size particles. Thus we consider particles whose charge and hence current distributions are given by

\[
\rho_j(\mathbf{x}) = q_j S(\mathbf{x} - \mathbf{x}_j) \tag{14}
\]

\[
\mathbf{j}_j(\mathbf{x}) = q_j \mathbf{v}_j S(\mathbf{x} - \mathbf{x}_j) \tag{15}
\]

where \( S(\mathbf{x}) \) is the shape factor which determines the distribution of charge of a finite-size particle. \( S(\mathbf{x}) \) may be positive and we assume it is normalized so that

\[
\int S(\mathbf{x}) \, d\mathbf{x} = 1 \tag{16}
\]

While the choice of \( S(\mathbf{x}) \) is arbitrary, one choice may be a gaussian shape,

\[
S(\mathbf{x}) = \frac{1}{(2\pi)^{3n/2}a^n} \exp\left[ -\frac{\mathbf{x}^2}{2a^2} \right] \tag{17}
\]

where \( n \) is the dimensionality (n=1,2,3). Here \( a \) is the size of the particle.

One immediate consequence of the use of such extended particles is the elimination of singularities at short distance while at long distance, little modification takes place. In fact when two particles of finite extent approach closer overlapping with each other, the force between the two becomes smaller and smaller. Thus we would expect short range collisional interaction will be greatly reduced. We must carefully estimate just how much modification to classical
plasma physics has been brought in by using such a model. We show in the following that long wavelength, collective plasma processes are little modified while short range collisional effects are greatly reduced.

2.3 Modification to Plasma Kinetic Theory Using Finite-size Particles

Let us consider what kind of modifications are necessary for a plasma of finite-size particles. For this purpose, we shall assume that the finite-size particles have no internal degree of freedom and furthermore they pass through with each other. The force on a particle centered at $(x, v)$ may be given by

$$ F(x, v, t) = q \int dx' S(x' - x) \left[ E(x', t) + \frac{1}{c} v \times B(x', t) \right]. \quad (18) $$

Charge and current densities for finite-size particles are given by

$$ \rho(x, t) = \int dx' S(x - x') \rho_\delta(x', t) \quad (19) $$

$$ J(x, t) = \int dx' S(x - x') J_\delta(x', t) \quad (20) $$

where $\rho_\delta$ and $J_\delta$ are charge and current densities for centers of finite-size particles defined by Eqs. (11) and (12). Since the above equations are of the form of convolution integral, they take a particularly simple form when transformed into Fourier space.

$$ F(k, v, t) = q \int \frac{d^3x}{(2\pi)^3} S(k, t) \left[ E(k, t) + \frac{1}{c} v \times B(k, t) \right] \quad (21) $$

$$ \rho(k, t) = S(k) \rho_\delta(k, t) \quad (22) $$

and

$$ J(k, t) = S(k) J_\delta(k, t) \quad (23) $$

where

$$ S(k) = \int dx S(x) \exp(-ik \cdot x). \quad (24) $$

Note $S(k)=1$ for point particles. Also $S(k=0)=1$. For gaussian particles where $S(x)=\exp(-x^2/(2a^2))/(2\pi)^{1/2}a$, $S(k)=\exp(-k^2a^2)/2$. "a" will give the "size" of particles in real space and $a^{-1}$ will be a measure of the spread in k-space. Generally speaking, $S(k)=1$ for $ka<1$ and $S(k)=0$ for $ka>1$. For square particles, $S(x)=1/\Delta x$ for $-\Delta x/2 < x < \Delta x/2$ and zero otherwise so that $S(k)=\sin(k\Delta x/2)/(k\Delta x/2)$ which becomes zero for particle wavelengths where $\sin(k\Delta x/2)=0$ is satisfied. In the following we shall assume the shape factor is symmetric. $S(k)=S(-k)$, which is satisfied for most of the simulation models.

2.4 Vlasov-Maxwell Equations

It is straightforward to write down a set of Vlasov-Maxwell equations for finite-size particles. Assuming $f(x,y,t)$ is the distribution function for the center of finite-size particles. Vlasov
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The equation is given by

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{F}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0 \]  

(25)

where \( F(\mathbf{x}, \mathbf{v}, t) \) is defined by Eq. (18). Charge and current densities are given by

\[ \rho(\mathbf{x}, t) = q \int d\mathbf{x}' d\mathbf{v} \ S(\mathbf{x} - \mathbf{x}') \ f(\mathbf{x}', \mathbf{v}, t) \]  

(26)

and

\[ \mathbf{J}(\mathbf{x}, t) = q \int d\mathbf{x}' d\mathbf{v} \ S(\mathbf{x} - \mathbf{x}') \ \mathbf{f}(\mathbf{x}', \mathbf{v}, t) \ \mathbf{v} \ . \]

Much of the plasma properties using finite-size particles may be studied from linear dispersion relation for small amplitude oscillations. Writing

\[ f(\mathbf{x}, \mathbf{v}, t) = f_0(\mathbf{v}) + f_1(\mathbf{x}, \mathbf{v}, t) \]  

(27)

where \( f_0(\mathbf{v}) \) is the zero-order equilibrium distribution and \( f_1 \) is a small perturbation, the Vlasov equation may be linearized in the absence of a d.c. magnetic field to find

\[ \frac{\partial f_1}{\partial t} + \mathbf{v} \cdot \frac{\partial f_1}{\partial \mathbf{x}} + \frac{F_1}{m} \frac{\partial f_0}{\partial \mathbf{v}} = 0 \]  

(28)

where

\[ F_1 = q \int d\mathbf{x}' \ S(\mathbf{x}' - \mathbf{x}) \ \mathbf{E}(\mathbf{x}') \]  

(29)

and

\[ \nabla \cdot \mathbf{E} = 4\pi q \int d\mathbf{x}' d\mathbf{v} \ S(\mathbf{x}' - \mathbf{x}) \ f_1(\mathbf{x}', \mathbf{v}, t) \ . \]  

(30)

Fourier analyzing in space and time, \( f_1 \), \( \mathbf{E} \sim \exp(ik\mathbf{x} - i\omega t) \), it is straightforward to write

\[ \left(-i\omega + ik\mathbf{v}\right) f_1 = -\frac{q}{m} S(\mathbf{x}) \ \mathbf{E}(\mathbf{k}) \ f_0 \]  

and

\[ i\mathbf{kE}(\mathbf{k}) = 4\pi q S(\mathbf{k}) \int d\mathbf{v} \ f_1(\mathbf{k}, \mathbf{v}, t) \]

so that the familiar plasma dielectric constant \( \varepsilon(k, \omega) \) is given by

\[ \varepsilon(k, \omega) = 1 - \frac{\omega_{pe}^2}{k^2} S^2(\mathbf{k}) \int \frac{f_0}{\omega - k\mathbf{v}} \ d\mathbf{v} \ . \]  

(31)

Note the only modification to the conventional dielectric constant for zero-size particles is the modification of \( \omega_{pe}^2 \) to \( \omega_{pe}^2 S^2(\mathbf{k}) \). This modification results from the reduction of the force \( \mathbf{F} \) between two finite-size particles. Since \( S(\mathbf{k}) \sim 1 \) for \( ka \gg 1 \), \( S(\mathbf{k}) \sim 0 \) so that the interactions in plasmas are greatly reduced. If \( a \) is chosen appropriately, one can eliminate the phenomena at wavelengths shorter
than $a$. One of such choices is to assume $a$ equal to the Debye length $\lambda_D$ since modes with $k\lambda_D > 1$ are often unimportant in a plasma. This does not necessarily mean "$a" cannot be much larger than $\lambda_D$ and in fact in some applications $a=(10-20) \lambda_D$ are chosen (Okuda et al., 1979). Detailed discussions on the modification of the dispersion relation for finite-size particle plasmas is found in Langdon and Birdsall (1970).

2.5 Collisions and Fokker-Planck Equations

We have seen that the use of finite-size particles reduced the interactions at wavelengths shorter than the size of a particle ",a". We therefore expect that the collisions in a plasma of finite-size particles can be reduced greatly if $a$ is chosen of the order of the Debye length $\lambda_D$. We also expect the reduction in particle collisions in a plasma of finite-size particles in three dimensions is more than in two dimensions. This is because the Coulomb force in three dimensions varies as $r^{-2}$ while it goes as $r^{-1}$ in two dimensions so that the effects of smoothing by the use of finite-size particles at short distance are more enhanced in three dimensions.

In order to study the reduction factor, let us first calculate the force and the potential between two bare particles of finite extent. Consider a situation where one particle is located at the origin while the other is located at $x$. The electric field of the potential due to the particle at the origin is given by

$$ V \cdot E = 4\pi q_1 S(x) $$

and the force on the second particle at $x$ is given by

$$ F = q_2 \int S(x - x') dx' $$

Fourier transforming Eqs. (32) and (33) and introducing the potential $V$ for the force $F$

$$ F = -\nabla V $$

we find

$$ V(k) = \frac{4\pi q_1 q_2 S^2}{k^2} $$

and

$$ V(x) = \frac{1}{(2\pi)^3} \int dk V(k) \exp(ik\cdot x) $$

where $n$ is the dimensionality. Note that

$$ V(x) \sim \frac{q_1 q_2}{a} $$

for $x < a$ so that the potential does not diverge even when the two particles overlap on top with each other so long as "$a" is finite.
When "a" is taken to be $\lambda_D$, one expects that the collisions must be greatly reduced as the particle interaction at a distance shorter than "a" is greatly reduced. More detailed calculations on the force and the potential is found in Okuda and Birdsal (1970).

It is straightforward to derive the Fokker-Planck equation for a plasma of finite-size particles (Langdon and Birdsal 1970, Okuda and Birdsal 1970). The collision operator is given by

$$\frac{\partial f}{\partial t}_{\text{coll}} = \frac{\omega_{pe}}{n\lambda_D^2} L \frac{\partial}{\partial y} \frac{\partial}{\partial y} \frac{y^2}{2} \int_{-\infty}^{+\infty} g \frac{1 - gg}{g^2} \left( \frac{\partial}{\partial y} - \frac{\partial}{\partial y} \right) f(y,t) f(y',t) \, dy \, dy' \tag{38}$$

where

$$g = y - y' \tag{39}$$

and

$$L = \int_{0}^{\infty} dK^2 \frac{S^4}{K^2 (1 + S^2 / K^2 \lambda_D^2)} \tag{40}$$

$I$ is a unit tensor. Note that all the necessary modification is contained in $L$ given by Eq.(40) so that the Fokker-Planck equation formally remains the same. This is because the velocity space is unmodified by the use of finite-size particles. For $S=1$ and no shielding, $I=2 \ln n\lambda_D^2$ and one recovers the familiar estimate of collisions

$$\frac{\partial f}{\partial t}_{\text{coll}} \sim \frac{\omega_{pe}}{n\lambda_D^2} \ln n\lambda_D^2 \, dy \, dy' \tag{41}$$

For a plasma of finite-size particles, $I$ is greatly reduced due to the appearance of $S^2$ when $a=\lambda_D$. Numerical integration in Eq.(40) reveals $I=0.1$ for $a=\lambda_D$ and $I=10^{-3}$ for $a=10\lambda_D$ for a gaussian particle. (Langdon and Birdsal, 1970; Okuda and Birdsal, 1970). Note that the corresponding values of $I$ for zero-size particles is $I=2\ln n\lambda_D^2 \sim 10$ so that a large reduction is achieved by adapting finite-size particles.

3. NUMERICAL METHODS USING FINITE-SIZE PARTICLES

3.1 Electrostatic Simulation Models

Let us consider finite-size particles with the gaussian form factor in one dimension so that $S(x) = \exp(-x^2/2a^2)/\sqrt{2\pi} a$ and $S(k) = \exp(-k^2a^2/2)$. We have shown that the short wavelength modes, $k|a|$, are heavily suppressed while leaving the long wavelength modes unmodified. This would reduce the particle collisions as we have shown already. It is clear from Eqs. (9) and (10) that the first step in plasma simulation is to calculate the force on a particle. This can be done in several ways. Note, however, that the number of long wavelength modes (collective modes) in a plasma is in general much smaller than the number of particles. In fact the ratio of the
number of collective modes to the number of particles is equal to the plasma parameter. We should therefore calculate the force on a particle from electric and magnetic fields rather than directly summing up the Coulomb force between two interacting particles. Such a pair-wise calculation would be prohibitively time consuming and should be avoided unless accurate information is required at short wavelengths.

Let us consider an electrostatic simulation model again. The electric potential \( \phi(x,t) \) is given by Poisson's equation

\[
\nabla^2 \phi = -4\pi \sum_j q_j S(x - x_j)
\]

Assuming periodic boundary conditions for \( \phi \) for simplicity, Eq. (42) is Fourier transformed into \( \vec{z} \)-space.

\[
\phi(\vec{k}) = \frac{4\pi}{k^2} S(\vec{k}) \sum_j q_j \exp(-i\vec{k} \cdot \vec{x}_j)
\]

where the Fourier transform of the form factor \( S(\vec{k}) \) is assumed to be the same for all the particles.

The force on a particle at \( x \), is given by

\[
F(x) = q_j \int S(x - x') E(x') \ dx'
\]

so that its Fourier transform is given by

\[
F(\vec{k}) = q_j S(\vec{k}) E(\vec{k})
\]

The force on a particle at \( x = x_1 \) is found by inverting Eq. (45) into \( x \)-space.

\[
F(x_1) = q_j \sum_k S(\vec{k}) E(\vec{k}) \exp(i\vec{k} \cdot \vec{x}_j)
\]

where

\[
E(\vec{k}) = ik \phi(\vec{k})
\]

It is clear from Eqs. (43) and (46), that the most time consuming part of the field calculations hinges on the evaluation of the phaser, \( \exp(ik \cdot x_j) \), since \( MN \) such operations are required at each time step. Here \( M \) is the number of the Fourier modes and \( N \) is the number of simulation particles. We will review several methods evaluating the phaser.

3.2 Spectral Method

In this method, only several Fourier modes are retained in the simulations and Eqs. (43) and (46) are calculated as they appear. Assuming the form of the electric field

\[
E(x) = \sum_{k_{\text{min}}}^{k_{\text{max}}} E(k) \exp(ikx)
\]
in one-dimension. Eq. (46) reduces to

$$ F(x_i) = 2q_i \sum_{k_{\text{min}}}^{k_{\text{max}}} \frac{S^2(k)}{k} \sum_j q_j \sin(k(x_j-x_i)) $$

$$ = 2q_i \sum_{k_{\text{min}}}^{k_{\text{max}}} \frac{S^2(k)}{k} [\sin(kx_i)\sum_{j=1}^{N} q_j \cos(kx_j) - \cos(kx_i)\sum_{j=1}^{N} q_j \sin(kx_j)] . $$

Note that $\Sigma \cos kx_j$ and $\Sigma \sin kx_j$ is independent of $i$ and therefore can be summed at once. Since there are $M$ Fourier modes to be retained, the total number of operations will be of the order of $MN$, much less than $N^2$ required for the pairwise calculation. Since the calculations of sine and cosine are time-consuming, one may make use of formulae of trigonometry such as $\sin 2k = 2 \sin k \cos k$, $\cos 2k = \cos^2 k - \sin^2 k$, and so on. Such a code has been developed and used to simulate a long plasma device but with only a few longest wavelength modes play important roles for the development of plasma turbulence (Cheng and Okuda, 1977).

3.3 Multipole Expansion Method

While the spectral method is accurate and faster than calculating the Coulomb force pairwise, it is not fast enough for large calculations, particularly in multi-dimensions, where the number of particles and the Fourier modes increases rapidly with the dimension. We should like to find a method which involves of the order of $(M + M)$ operations rather than $MN$. This is done by introducing a spatial grid as shown below.

Consider again Poisson's equation in $k$-space.

$$ k^2 \phi(k) = 4\pi S(k) \sum_j q_j \exp(-ik \cdot x_j) . $$

Since we have already given up the exact representation of particle location by adapting the use of finite-size particles, it appears reasonable to replace the phasor $\exp(-ik \cdot x_j)$ by using an approximate particle location. This is done by using a spatial grid. Let us now consider a spatial grid and write the particle location

$$ x_j = n_j \Delta + \delta x_j $$

where $n_j$ is a set of integers representing the nearest grid point of the $j$-th particle and $\delta x_j = x_j - n_j \Delta$ is the displacement. $\Delta$ is the size of a spatial grid and need not be the same in each direction although we assume it is the same here for simplicity. Now the phase factor in Poisson's equation may be expanded about the nearest grid point. Poisson's equation is now written as

$$ k^2 \phi(k) = 4\pi S(k) \sum_j q_j \exp(-ik \cdot n_j \Delta) [1 - ik \cdot \delta x_j - \frac{(k \cdot \delta x_j)^2}{2!} + \cdots ] . $$

Summation over the particles can be replaced by the summation over the grid point so long as the particles have the same nearest grid point. For example.
\[
\sum_{j=1}^{N} q_j \exp(-i k \cdot n_j \Delta) = \frac{1}{n} \left( \sum_{j \in \mathbb{Z}} q_j \exp(-i k \cdot n_j \Delta) \right) = \sum_{n=1}^{N} q_{n} \exp(-i k \cdot n \Delta) \quad (52)
\]

where \( q_n = \sum_{j \in \mathbb{Z}} q_j \delta(x_j) \) is the net charge (monopole) at the \( n \)-th grid point. Similarly,

\[
\sum_{j=1}^{N} q_j \exp(-i k \cdot n_j \Delta) = \frac{1}{n} \sum_{n=1}^{N} q_{n} \exp(-i k \cdot n \Delta) \quad (53)
\]

where \( q_n = \sum_{j \in \mathbb{Z}} q_j \delta(x_j) \) is the net displacement (dipole) of the charges at the \( n \)-th grid point. One can continue the expansion to higher orders if necessary. Noting that the wavenumber is given by \( k = 2 \pi n / L \) for a periodic system, Eqs. (52) and (53) correspond to discrete Fourier transforms defined by

\[
\hat{g}_m = \frac{1}{L} \sum_{n=1}^{N} g_n \exp(-i 2 \pi m n / L) \quad (54)
\]

whose inverse Fourier transform is given by

\[
g_n = \frac{1}{L} \sum_{m=1}^{N} \hat{g}_m \exp(i 2 \pi m n / L) \quad . \quad (55)
\]

The force on a particle at \( x_j \) is calculated similarly as

\[
F(x_j) = q_j \sum_k \sum_k \sum_{m=1}^{N} E(k) S(k) \exp(i k \cdot x_j) \exp(-i k \cdot n_j \Delta) \exp(i k \cdot \delta x_j) \quad (56)
\]

where the first term of Eq. (56) is the force on a particle at the nearest grid point and the second term is the correction due to dipole moment associated with the gradient of the field. The number of operations associated with the multipole expansion is only proportional to the number of particles for the charge density and force calculations (Kruer et al., 1973). In addition, the number of operations associated with the discrete Fourier transform scales as \( M \ln M \) where \( M \) is the number of Fourier modes. It is shown that the higher order terms associated with the expansions given by Eqs. (51) and (56) converge rapidly so that under normal circumstances one can truncate at the dipole term (Chen and Okuda, 1975; Okuda and Cheng, 1978).

One of the drawbacks of the multipole expansion method is that it requires several arrays for storing field quantities. For example, for two-dimensional electrostatic simulations, three two-dimensional arrays are necessary for charge density up to the dipole moments. For the electric field calculations, we must store \( E_x, E_y, \delta E_x/\delta x, \delta E_x/\delta y, \) and \( \delta E_y/\delta y \). Note for electrostatic simulations \( \delta E_x/\delta x = \delta E_y/\delta y \). For three-dimensional simulations or electromagnetic simulations, the number of arrays required can often exceed the capacity of available
computers. It is important to keep the number of the field arrays to the minimum in order to be able to perform large scale, multi-dimensional simulations. This is because the field arrays or grid quantities are randomly accessed for the calculation of charge density and force on a particle so that it is desirable to store the field arrays in the central memory of a computer rather than in an auxiliary memory such as disks and tapes. It is often necessary, on the other hand, to store particle data (positions and velocities) on disks and tapes in order to be able to use large number of particles. In this case, only a small fraction of particles are brought into the central memory of a computer for the calculations of charge density and force and they are sent back to the outside memory after such calculations. We now consider another simulations method where interpolations of charge and force on the grid points are used. Such a method is often called PIC (particle-in-cell) (Morse and Nielson, 1969) and CIC (cloud-in-cell) (Birdsall and Fuss, 1969) methods.

3.4 Interpolations and Weighting

The lowest order interpolation for charge or force is equivalent to the monopole approximation in which the entire amount of charge is assigned to the nearest grid point (NGP). Similarly the force on a particle is approximated by that at the nearest grid point. Schematically NGP weight function may be sketched as shown in Figure 1(a) where for particle location x with $-\Delta/2 < x < \Delta/2$, the entire charge or force is assigned at the nearest grid point. Therefore the weight function $w_0$ is given by

$$w_0(x) = \begin{cases} 1/\Delta & \text{for } -\Delta/2 < x < \Delta/2 \\ 0 & \text{otherwise} \end{cases} . \quad (57)$$

In this case the particles appear to have a shape of a slab in the NGP interpolation with the width of $\Delta$.

In the next approximation, charge on a particle is linearly interpolated between two nearest grid points as shown in Figure 1(b) so that its weight function is given by

$$w_1(x) = \begin{cases} (x + \Delta)/\Delta^2 & \text{if } -\Delta < x < 0 \\ (-x + \Delta)/\Delta^2 & 0 < x < \Delta \\ 0 & \text{otherwise} \end{cases} . \quad (58)$$

It is interesting to observe that the Fourier tranform of the weight function is given by

$$w_n(k) = [\sin(k\Delta x/2)/(k\Delta x/2)]^{n+1} \quad (59)$$

so that $w_n(k=0)=1$ for any $n$. For large $n$, $w_n(k)$ is unity near $k\Delta x=0$ and nearly zero otherwise. For $n=3$, the weight function is given by
as shown in Figure 1(c) and this interpolation is sometimes called the quadratic spline. It is clear that the higher order interpolations involve operations including more grid points in \( x \)-space so that its

\[
\begin{align*}
W_3(x) &= \begin{cases} 
\frac{3}{4} - \frac{x^2}{\Delta^2}, & 0 < \frac{x}{\Delta} \leq 1/2 \\
\frac{1}{4} - \frac{|x|\Delta + (x\Delta)^2}{\Delta^3}, & 1/2 < \frac{x}{\Delta} \leq 1 \\
0, & \text{otherwise}
\end{cases}
\end{align*}
\]

(60)

Figure 1. Weighting functions of charge density at the nearest grid point for the nearest grid point (a), linear interpolation (b) and quadratic interpolation (c).

Fourier transform is more and more narrowly peaked for \( k\Delta x \rightarrow 0 \) which reduces numerical aliases (Langdon, 1971; Okuda et al., 1979). In general, the interpolation for the charge density takes the form of

\[
p_n^D = \sum_j q_j w(x_n - x_j)
\]

(61)

where \( p_n^D \) is the charge density at the \( n \)-th grid point, \( w \) is the weight function and \( x_n \) is the \( n \)-th grid point. Similarly, the force on a particle is given by
F(x_j) = q_j \sum_n E_n w(x_n - x_j). \quad (62)

Since the charge density and electric field are defined only on a set of discrete grid points, a set of Fourier modes

\[ k_p = k \pm pk_g \quad (p = 0, 1, 2, 3, \ldots) \]

will give the same variation in x where \( k_g = 2\pi/\Delta \) is the grid wave number. Detailed analysis of such algorithms reveals a presence of numerical instabilities associated aliases (\( p \neq 0 \)) when the Debye length is much smaller than the grid size (Langdon, 1971; Chen and Okuda, 1975). Such numerical instabilities may be quenched by employing a higher order interpolations which reduces the amplitude of the aliases (Okuda and Cheng, 1978; Okuda et al., 1979).

3.5 Finite Difference Equation

Let us now consider the left-hand-side of the equation of motion as given by Eqs. (9) and (10). The problem here is how to approximate the differential equation by the finite-difference equation. The difference equation must be simple so that it can be integrated fast and yet at the same time it must be reasonably accurate after many iterations.

We consider again the electrostatic model in which the force on a particle is determined only from the particle location.

\[
m_j \frac{dv_j}{dt} = q_j E[x_j(t)] \quad (63)
\]

\[
\frac{dx_j}{dt} = v_j(t)
\]

The standard method for this case is the leap-frog scheme in which particle positions and velocities are defined at two different sets of time steps shifted by \( \Delta t/2 \). It is given schematically by

\[
\frac{v^t - v^t - \Delta t}{\Delta t} = q_j \frac{m_j}{E^t - \Delta t/2}
\]

\[
\frac{x^{t+\Delta t/2} - x^{t-\Delta t/2}}{\Delta t} = v^t
\]

(64)

It is clear that the leap-frog scheme is time-centered and is reversible in time regardless of the size of the time step \( \Delta t \). The accuracy of the leap-frog scheme may be estimated by Taylor expanding \( v^t \) and \( v^t - \Delta t \) at around \( v^t - \Delta t/2 \). We find \( v^t - v^t - \Delta t = v^t - \Delta t^3/24 \) so that the error per time step will be of the order of \( (\omega \Delta t)^3/24 \), giving \( 10^{-3} \) to \( 10^{-4} \) for \( \omega \Delta t = 0.1 \) to 0.2 which are commonly used. Note the leap-frog scheme is particularly simple and requires storage for \( v \) and \( x \) only at one time step since the new \( v \) and \( x \) replace those
in the past step.

In order to consider stability, let us examine a harmonic oscillator in one-dimension where the equation motion takes the form of

$$\frac{d^2x}{dt^2} = -\omega_0^2 x$$  \hspace{1cm} (65)

The general solution to Eq. (65) is given by

$$x(t) = c_1 \cos \omega_0 t + c_2 \sin \omega_0 t$$ \hspace{1cm} (66)

where $c_1$ and $c_2$ are determined from the initial position and velocity of the particle. The corresponding leap-frog scheme is given by

$$\frac{x^{t+\Delta t} - 2x^t + x^{t-\Delta t}}{\Delta t^2} = -\omega_0^2 x^t$$ \hspace{1cm} (67)

The stability is found by assuming $x^t = \exp(i\omega t)$ to find

$$\sin(\omega \Delta t/2) \pm \omega_0 \Delta t/2$$ \hspace{1cm} (68)

It is clear that for a large $\Delta t$ satisfying $\omega \Delta t > 2$, there is no real solution to $\omega$ and the leap-frog scheme is unstable (Birdsall and Langdon, in press). Since the numerical error is of the order of $(\Delta t)^3$ in the leap-frog scheme, one can reduce $\Delta t$ in order to improve the accuracy of the computation for the same length of integration.

Another important application of the leap-frog scheme is the equation of motion in a static uniform magnetic field where Eq. (63) is replaced by the Lorentz force,

$$\frac{dv}{dt} = \frac{q}{m} (\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B}_0)$$ \hspace{1cm} (69)

The time-centered, leap-frog scheme may be written as (Buneman 1967)

$$\frac{\mathbf{v}^{t+\Delta t/2} - \mathbf{v}^{t-\Delta t/2}}{\Delta t} = \frac{q}{m} \left( \frac{\mathbf{E}}{\Delta t} + \frac{1}{c} \frac{\mathbf{v}^{t+\Delta t/2} + \mathbf{v}^{t-\Delta t/2}}{2} \times \mathbf{B}_0 \right)$$ \hspace{1cm} (70)

where the velocity $\mathbf{v}^t$ at the right-hand-side is replaced by the average of $\mathbf{v}^{t+\Delta t/2}$ and $\mathbf{v}^{t-\Delta t/2}$. It is straightforward to prove that Eq.(70) conserves particle energy in the absence of the electric field.

$$\mathbf{v}^{t+\Delta t/2} = \mathbf{v}^{t-\Delta t/2}$$

regardless of the size of $\Delta t$. This is proven by multiplying $(\mathbf{v}^{t+\Delta t/2} - \mathbf{v}^{t-\Delta t/2})$ to both sides of Eq. (70). This is reasonable since the effect of $\mathbf{B}_0$ is to rotate particle velocity around $\mathbf{B}_0$. Since Eq.(70) is an algebraic equation with respect to $\mathbf{v}$, one can solve for $\mathbf{v}^{t+\Delta t/2}$ to find
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\[
\begin{align*}
\tilde{v}_t^+\Delta t/2 &= \frac{1-(\omega_c\Delta t/2)^2}{1+(\omega_c\Delta t/2)^2} \tilde{v}_t^-\Delta t/2 - 2x\tilde{v}_t^-\Delta t/2 \frac{\omega_c\Delta t}{1+(\omega_c\Delta t/2)^2} \\
&+ \frac{q\Delta t}{m} \frac{\vec{E}}{1+(\omega_c\Delta t/2)^2} + \frac{q^2\Delta t^2}{2m^2c} \frac{\vec{E} \times \vec{B}_0}{1+(\omega_c\Delta t/2)^2}.
\end{align*}
\] (71)

Boris has shown that Eq. (71) can be obtained by adding the electric field acceleration of the particle velocity by \(\Delta t/2\) time step, and a full rotation by the magnetic field accompanied by another \(\Delta t/2\) step electric acceleration (Boris 1970). This can be seen by rewriting Eq. (70) as

\[
\tilde{v}_t^+\Delta t/2 - \tilde{v}_t^-\Delta t/2 + \tilde{x} \omega_c \Delta t/2 = \tilde{v}_t^-\Delta t/2 + \tilde{x} \omega_c \Delta t/2 + \frac{q}{m} \vec{E} \Delta t.
\] (72)

where \(\omega_c = qB_0/mc\) (Dawson, 1983). Eq. (72) is written as

\[
\vec{R}(-\theta \Delta t/2) \tilde{v}_t^+\Delta t/2 = \vec{R}(\theta \Delta t/2) \tilde{v}_t^-\Delta t/2 + \frac{q}{m} \vec{E} \Delta t
\]

where \(\vec{R}\) is a rotation matrix about the magnetic field for an angle \(\theta \Delta t/2\). Taking \(\vec{B}_0\) in the \(\vec{z}\) direction, \(\vec{R}\) is found

\[
\vec{R} = \begin{bmatrix}
\cos(\theta \Delta t/2) & -\sin(\theta \Delta t/2) & 0 \\
\sin(\theta \Delta t/2) & \cos(\theta \Delta t/2) & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

with \(\tan(\theta \Delta t/2) = \omega_c \Delta t/2\) (Buneman 1967). Solving for \(\tilde{v}_t^+\Delta t\) gives

\[
\tilde{v}_t^+\Delta t/2 = \vec{R}(\theta \Delta t) \tilde{v}_t^-\Delta t/2 + \frac{q}{m} \vec{R}(\theta \Delta t/2) \cdot \vec{E} \Delta t.
\] (73)

3.6 Guiding Center Model and Predictor-Corrector Method

One of the dynamical systems in which the leap-frog scheme cannot be applied is the guiding center model. In this model, fast gyration around magnetic field lines is averaged out so that only the slow drift motion of guiding centers is followed in time. Clearly the frequency of the physical process involved must be smaller than the gyro-frequency, \(\Omega\), and at the same time the wavelength of the variation of physical quantities must be longer than the gyroradius.

Let us consider, for example, a two-dimensional guiding center model in which a plasma is embedded in a uniform strong magnetic field in \(\vec{z}\)-direction. Such a plasma may be regarded as two-dimensional since the motion along magnetic field quickly smooths out any variations along magnetic field while the motion across it is much slower. Particle motion may be described by its guiding center drift due to electric field given by \(cE/\vec{B}^2\). The equation of motion would be
\[
\frac{dx}{dt} = \frac{C}{B} E_y(x) \\
\frac{dy}{dt} = -\frac{C}{B} E_x(x)
\]

where only the first order time derivatives appear so that the leapfrog scheme cannot be applied here. One can try a leap frog scheme by stepping two time steps at once as shown below.

\[
x^{n+1} = x^{n-1} + 2\Delta t \frac{C}{B} E_y^n \\
y^{n+1} = y^{n-1} - 2\Delta t \frac{C}{B} E_x^n
\]

One of the problems using such a scheme is that "even" and "odd" time steps are coupled only through the electric field, so that particle positions at even and odd steps are found to diverge as the iterations are repeated in time. It is therefore necessary to average the even and odd steps as frequently as possible. Such a scheme is called a predictor-corrector method. In the predictor step, the same equation is used.

\[
x^{n+1*} = x^{n-1} + 2\Delta t \frac{C}{B} E_y^n \\
y^{n+1*} = y^{n-1} - 2\Delta t \frac{C}{B} E_x^n
\]

where \((x^{n+1*}, y^{n+1*})\) is the predicted value. In the corrector step,

\[
x^{n+1} = x^n + \Delta t \frac{C}{B} (E_y^n + E_y^{n+1*})/2 \\
y^{n+1} = y^n - \Delta t \frac{C}{B} (E_x^n + E_x^{n+1*})/2
\]

are used to find \((x^{n+1}, y^{n+1})\) where \(E^*\) is the electric field determined from the predicted positions, \((x^*, y^*)\). Such a scheme gives satisfactory results for the simulations of the guiding center model in which low frequency particle motion across magnetic field has been studied with respect to turbulent diffusion associated with microinstabilities (Lee and Okuda, 1978).

The example given here is one of the simplest equations of motion. Particle drifts such as due to magnetic field gradient, magnetic field curvature and external force may be added to the \(cE_xB/B^2\) drift in a similar manner.

**3.7 Quasi-neutral Particle Simulation Model**

The guiding center model describes the slow motion of a plasma across magnetic field assuming a plasma quickly becomes uniform along magnetic field by the rapid thermal motion along the field lines. When such a rapid motion along magnetic field must be considered, it is necessary to use a small time step determined from the electron motion.
along magnetic field lines. When considering low frequency ion waves such as ion acoustic, ion cyclotron and drift waves, there are situations in which detailed electron motion in phase space may not be essential. Of course, there are certainly cases where precise electron dynamics is crucial especially when considering microinstabilities driven by the electron Landau damping.

Here we consider a model for studying ion waves in which detailed electron motion is not necessary. In particular we would like to drop electron inertia since it is responsible to generate high frequency electron plasma oscillations. In the presence of low frequency waves where the phase speed of the wave along magnetic field, \( \omega / k_B \), is much smaller than the electron thermal speed, \( v_T \), electron response may be approximated by the Boltzmann distribution

\[
\psi = n_0 \exp(\psi/T_e) .
\]

Poisson's equation for the system is given by

\[
\psi^2 \psi = -4\pi \exp(\psi/n_1 - n_0 \exp(\psi/T_e)) .
\]

so that for \( \psi/T_e \ll 1 \), we may expand \( \exp(\psi/T_e) \approx 1 + \psi/T_e \) obtaining

\[
\psi^2 \psi = -4\pi \frac{n_0 + \psi}{T_e} + 4\pi \frac{n_0}{T_e} \cdot \psi
\]

For a uniform plasma, \( n_0 \) and \( T_e \) are constants so that Poisson's equation is Fourier transformed in k-space after substituting \( n_1 = n_0 + \delta n_1 \), finding

\[
\phi_k = \frac{4\pi e \delta n_1}{k^2 + \omega^2}
\]

in which the electrons appear as the Debye shielding cloud of the potential around the ion charge density. It is not necessary therefore to calculate electron density in this model. It should be noted that the simulation model using the technique just described is not only much faster than the conventional electron-ion model but also it is much quieter because of the absence of high frequency electron plasma waves (Okuda et al., 1978).

when a plasma is inhomogeneous in one-direction,

\[
n_e(x) = n_0(x) [1 + e\phi(x)/T_e]
\]

so that, with \( n_0(x) = \bar{n}_0 + \delta n_0(x) \), Poisson's equation takes the form of

\[
\psi^2 \psi = -4\pi e \bar{n}_0 \psi + \frac{4\pi e \delta n_0}{T_e} \psi
\]

This equation may be solved by iteration about \( \bar{n}_0 \) in which, for the first iteration, \( \delta n_0 \) term is neglected to find \( \psi \). In the next iteration \( \delta n_0 \) term is back to obtain a new potential.

So far, we have treated the electrons in the adiabatic limit in
which no resonant wave-particle interactions are taken into account. There are, however, occasions where small non-adiabatic electrons may play an important role in controlling microinstabilities in a collisionless plasma. In order to recover the resonant wave-particle interactions, we must follow electrons in velocity space so that electrons are no longer considered a fluid. Unfortunately, however, as soon as the electrons recover their discreteness and inertia, high frequency plasma oscillations appear and the advantages gained from the adiabatic electron model vanish. There are several techniques to cure the situation, however, they are of limited use and there is no model which works for general purpose.

One of the models is to recognize that the resonant electrons with the waves are low energy electrons satisfying \( \omega / k_\parallel < v_e \) so that one may divide the total electron velocity distribution into resonant and non-resonant particles. For non-resonant particles, Boltzmann distribution should be applied while the resonant particles whose velocity is much less than the thermal speed are treated as discrete particles and their orbits in phase space are followed in time. Since the low energy electrons move slowly, it is possible to use a large time step, larger than \( v_e / \omega_{pi} \).

Poisson's equation may be written as

\[
\left( k^2 + k \cdot \partial \right) \phi_k = 4 \pi e \left( n_i - n_e^R \right)
\]

where \( n_e^R \) is the density from the resonant electrons. Such a model has been used to study, for example, ion acoustic instability in one-dimension. One of the questions naturally arises is the choice of the boundary between resonant and non-resonant particles. Obviously some of the resonant electrons do diffuse in velocity space as a result of quasilinear diffusion so that they may appear in the non-resonant region in velocity space. If that happens, those particles start emitting high frequency plasma waves so that such particles must be removed from the computation. There are other kind of models in which, for example, electrons are treated as a massless fluid with macroscopic density, velocity, temperature and so forth (Sgro and Nielson, 1976).

3.8 Initial Conditions

Before starting a simulation, one must specify initial conditions in phase-space. This is ordinarily done by specifying particle distribution functions at \( t=0 \). This may appear simple so long as we know what we want to simulate. The choice of initial conditions, that is to assign the initial position and velocity to each simulation particle is not as simple as it appears. This is because the initial condition is often given by a particle distribution function in phase space, \( f(x,v,t=0) \), while only a finite number of particles or degree of freedom is available to represent the initial distribution.

Consider, for example, a Maxwellian plasma in a uniform plasma in one-dimension. In order to represent a uniform distribution in space,
one might load particles exactly uniformly along the $x$ axis with equal spacing, or one might load particles randomly using a uniform random number generator. Certainly there are many other ways of choosing the initial positions. There is no way of deciding which one is the best in general. It all depends on the problem under consideration. If one is interested in, for example, a coherent wave in a plasma, exact uniform spacing of particle positions might be better. If, on the other hand, one is interested in turbulence where many modes are present, then uses of random numbers might give a better choice. Similar statement can be made for a velocity space distribution.

Among many different ways of initial loading, the quiet start in which the phase space is loaded as uniformly as possible has interesting characteristics (Byers and Grewal, 1970). For a spatially uniform Maxwellian, for example, quiet start can be obtained by loading particles uniformly in $x$ and repeating the velocities used to represent a Maxwellian velocity distribution at one location in $x$ for all the values of different $x$. In this way, uniform phase space is maintained and there would be no random noise associated with the initial loading. Such a loading scheme can be used for any distribution which is uniform in the coordinate space. If a plasma is intrinsically unstable with respect to plasma instabilities, initial noise associated with machine round-offs will grow to large amplitude until limited by nonlinear effects.

Clearly the advantage of using a quiet start is to suppress the unwanted noise coming from the initial loading such as the one associated with the use of random numbers and therefore the quiet start is particularly useful when studying weak instabilities or small amplitude phenomena. When studying strong instabilities or large amplitude phenomena, differences arising from different initial loadings are expected small.

There are several short-comings associated with the quiet start. However, one obvious drawback is that the method cannot be applied in general to a nonuniform plasma. The other drawback, which is more fundamental, is the presence of multi-beam instability in the presence of beams associated with the quiet start. Quiet start may be considered to consist of an ensemble of cold beams whose distribution is given by

$$ f = \sum_i n_i \delta(v - v_{bi}) $$

(79)

Instabilities arising from the presence of multi-beams have been studied in detail (Dawson, 1960) and it is shown that the growth rate is proportional to $k \delta v$ where $\delta v$ is the spacing of the beam. By choosing the sufficient number of beams, the growth rate may be reduced to a much smaller value compared with the growth rate of the physical instability one is looking for. If that is the case, beam instability associated with the presence of multi-beams may be harmless.

Another interesting trick in plasma simulations useful when a
small region in phase-space play an important role in particle weighting. Such an example is the well-known bump-on-tail instability in which a weak electron beam is injected to a background thermal plasma. Here the beam density, \( n \), can be as small as 1% of the background density \( N \), so that most of the particles may be used to represent the bulk distribution where little physics takes place. Most of the nonlinear effects such as particle trapping occur on beam particles where there are only a small fraction of simulation particles representing them.

It is possible to choose \( n \sim N \) so that statistical fluctuations associated with the small number of beam particles do not mask the physics one is trying to study. If \( n \sim N \) is chosen, then one must assign smaller charge and mass to beam particles while keeping \( q/m \) unchanged. It is clear that so long as \( q/m \) stays the same, Vlasov equation or equation of motion remains the same. The only change in the simulation code is in the charge density calculation in which beam particles carry smaller amounts of charge. It may be pointed out that while Vlasov equation remains the same, collisional effects associated with the two-body correlation will be modified even if \( q/m \) is kept unchanged.
PART II: Application of Particle Simulation to Electrostatic Ion Cyclotron Waves on Auroral Field Lines

1. INTRODUCTION

It is well known that the electrostatic ion cyclotron (EIC) waves may be destabilized by drifting electrons (current) through the stationary ions (Drummond and Rosenbluth, 1962; Kindsel and Kennel, 1971; Okuda et al., 1981). EIC waves are particularly important in an isothermal plasma \((T_e = T_i)\) where the ion acoustic waves may be stable due to Landau damping. The threshold drift speed is a fraction of electron thermal speed so that EIC waves may easily be excited either by a current or an ion beam.

Laboratory experiments as well as space craft measurements have been reported recently on the observation of EIC waves in tokamaks (TFR Group, 1978), linear devices (Yamada and Hendel, 1978), and space plasmas (Kintner et al., 1979; Yau, et al., 1983). Large amplitude density fluctuations, heating of ions across magnetic field and anomalous cross-field particle diffusion have been observed in these measurements.

There are a number of theoretical considerations on the linear as well as nonlinear behavior of the current-driven EIC instabilities. Linear theory predicts that the unstable modes satisfy

\[
\omega \propto n \Omega_i \\
k_i \rho_i \propto n
\]

(80)

where \(\rho_i\) is the ion thermal gyroradius and \(n\) is an integer representing a cyclotron harmonic.

When the electron drift speed is above the threshold, EIC waves grow to large amplitude until limited by nonlinear effects. In the absence of electron source, plateau formation on the electron distribution due to quasilinear diffusion gives rise to the nonlinear saturation of the EIC waves resulting in a modest ion heating (Drummond and Rosenbluth, 1962). There are situations, however, in which a flux of fresh electrons constantly replenishes the distribution function of electrons so that complete stabilization due to plateau formation cannot take place. Plasma heating experiments by injection of electron beams (Yamada and Hendel 1978), ion beams (Eubank et al., 1979) and field-aligned auroral currents where the ionosphere acts as a reservoir of fresh electrons are such examples. For these cases, the duration of beams is much longer than the characteristic time scale of the EIC waves so that a presence of beam source plays an important role on the nonlinear behavior of the EIC waves. Ion heating and plasma transport.
Here we would like to present results from numerical simulations on EIC waves with and without a presence of source. Numerical results obtained from the initial value simulations without a plasma source are given in Sec.2. In Sec.3, we present simulation results in which a plasma is subject to electron beam injection at one end of the system. In Sec.4, the simulations are extended to two dimensions where large amplitude density striations across magnetic field appear. These density striations may be responsible for the generation of auroral are elements.

2. RESULTS OF SIMULATIONS WITHOUT A SOURCE

In this Section, we shall present results obtained from one- and two-dimensional numerical simulations on the EIC instabilities. The simulation model used is an electrostatic model in which full dynamics is retained for the ion motion while guiding center drift approximation is used for the electrons. This approximation for the electrons is valid for low frequency, $\omega \ll \Omega_e$, and long wavelength, $k_i \rho_e \ll 1$, oscillations where electrons are treated as guiding center particles. Electron motion along magnetic field is solved exactly. In essence, a set of equations for this model are

$$m_i \frac{dv_i}{dt} = e \left( E(x_i) + \frac{1}{c} v_i \times B \right)$$

$$m_e \frac{dv_e}{dt} = -e E_e(x_e)$$

$$v_{ie} = \frac{cE(x_e) \times B}{B^2}$$

$$\frac{dx_i}{dt} = v_i$$

$$\nabla^2 \phi = -4\pi e (n_i - n_e)$$

$$E_e = -\nabla \phi$$

which have been solved on a spatial grid using a finite difference integration in time (Lee and Okuda, 1978).

The initial conditions for particles are a stationary Maxwellian for the ions and a drifting Maxwellian for the electrons along magnetic field. Initially, spatial distribution is uniformly loaded using random numbers. The parameters of the simulations are $m_i/m_e=1837$, $\omega_{pe}/\Omega_e=0.2$ and $T_e=T_i$ initially.

Let us first study results obtained from a one-dimensional
simulation in which a uniform magnetic field is taken in the y-z plane with \( B_y/B_z = 0.1 \). Perturbations are allowed only in the y-direction (one-dimensional model). \( \nu_{de}/\nu_{te} = 1.4 \), \( L = 1024 \Delta \) where \( L \) is the system length and \( \Delta \) is the mesh size and \( \lambda_e = \Delta \). The allowed wavelengths on the grid points in this system is given by

\[
k_m = \frac{2\pi m}{L} \quad (m = 0, \pm 1, \pm 2, \ldots, \pm \frac{L}{2})
\]

so that \( k_e \rho_i \) varies 0.05 to 10 with the spacing \( \delta(k_e \rho_i) = 0.05 \). 70,000 ions and electrons are used which gives about 70 particles per grid for each species.

---

Figure 2. Time history of the real and imaginary parts of the potential, \( e\Phi_k(t)/T_e \), and its frequency for the 3rd (a) and the 23rd harmonics (b).
Figures 2 (a) and (b) indicate the time history of the real and imaginary parts of the electrostatic potential, $e\Phi_k(t)/T_e$, for the third mode (a), and the 23rd mode and their frequency spectrum (b). For the third mode, $k_\perp a = 0.16$, only the fundamental cyclotron harmonic is excited while for the 23rd mode, $k_\perp a = 1.2$, several harmonics are clearly seen. The amplitude for these modes reaches $e\Phi_k/T_e = 0.2$ before saturation.

![Figure 3. Electron velocity distribution along magnetic field at different times. Note the development of a plateau.](image)

Nonlinear saturation takes place when the electron velocity distribution develops a plateau as shown in Figure 3. At $\Omega_i t = 10$, a plateau is formed for the region of velocity space, $v < v_{de}$, which then creates a positive slope $\partial f_e/\partial v_\parallel > 0$ for $v > v_{de}$ as seen in Figure 3. This new region of the positive slope is flattened later as the long wavelength modes corresponding to larger phase velocity are destabilized.
Heating of ions perpendicular to magnetic field and the loss of electron kinetic energy along magnetic field is shown in Figure 4. The relative change for both ions and electrons remains small as discussed in Sec. 3 because the plateau formation on the electron distribution releases only a fraction of electron kinetic energy.

![Figure 4. Heating of ion perpendicular energy and cooling of electron kinetic energy along magnetic field.](image)

Simulations are extended to 2-dimensions in which spatial variations are allowed in the x-y plane with the external magnetic field oriented as before. Results of 2-dimensional simulations is expected to reveal processes not allowed in one-dimensional results such as mode-coupling among modes at different angles of propagation and cross-field particle diffusion across magnetic field.

Figure 5 shows a plot of test particle positions at an instant of time $\Omega_i t=30$, for electrons (top) and ions (bottom) which were initially located at a narrow strip located at $x=20$. The spread in the x-direction suggests the presence of cross-field particle diffusion due to the ion cyclotron instabilities. The measured diffusion coefficient, $D_x = \langle (\Delta x_e)^2 \rangle / t \approx 5 \times 10^{-3} \Delta^2 \omega_{pe}$ suggesting a presence of large anomaly for the transport coefficients associated with ion cyclotron waves.
Figure 5. Plot of the test particle positions at $Q_1 t = 30$ for electrons (top) and ions (bottom) which were initially located at $x = 20$. 
3. RESULTS OF SIMULATIONS WITH A SOURCE

We have seen earlier in Sec. 2 that the ion cyclotron instabilities saturate at a low level giving rise to a modest heating of ions in the absence of electron source. Here we present results of simulations obtained using a model in which a plasma is subject to a source which constantly injects electrons into a plasma system with the initial drifting Maxwellian velocity distribution as show in Figure 6. Such a model may represent an electron beam injection experiment.

![Figure 6. Theoretical model for auroral field lines in which the ionosphere is the source of cold, drifting Maxwellian electrons.](image)

in a plasma or an auroral current along magnetic field driven by the ionosphere-magnetosphere coupling (Okuda and Ashour-Abdalla, 1983). It is clear that the ion heating in this case is expected to be much stronger in the presence of an electron source due to the inhibition of plateau formation on the electron distribution function.

Figure 7 shows the profiles of ion density normalized by the average density for the entire system length plotted at three different times. The parameters of the simulations are the same to the one-dimensional simulations reported in Sec. 2 with \( L = 1024 \Delta \).
$v_{de} = 1.4v_{te}$, $m_i/m_e = 1837$, $k_z/k_i = 0.1$ and $\Omega_e/\omega_{pe} = 5$. The dashed vertical lines denote the boundary lines for different bins for diagnostic purposes. At time $\Omega t = 110$ (upper panel), the larger density perturbations, $\delta n/n = 0.25$ are mostly confined to the first two bins. At later times shown in the middle and lower panels, the ion density perturbations are seen to propagate and extend further right, suggesting the unstable EIC waves can propagate with the beam. From Figure 7, one can estimate the propagation speed along magnetic field to be $0.007v_{de}$. This speed is much smaller than the electron drift speed and is in good agreement with the self-induced propagation speed calculated theoretically (Okuda and Ashour-Abdalla, 1983).

Figure 7. Ion density profile at three different steps. Note a large density perturbation propagates along magnetic field.
The fact that the density modulation is associated with the ion cyclotron waves is confirmed by measuring the frequency at several different locations along field lines. This is shown in Figure 8 where the time history of electron density at two different locations, x=320A and x=416A are shown in the upper panel (a), while in the lower panel (b), frequency spectra of the density fluctuations are shown. The frequency analysis confirms the presence of coherent peaks above Q_i. In addition, there are much smaller, but clearly coherent peaks near ω=k_i c_s indicating oblique ion acoustic waves propagating nearly perpendicular to magnetic field.

![Figure 8](image_url)

Figure 8. Temporal behavior of the electron density perturbation at x=320A and x=416A and its frequency spectrum.

The effects of ion cyclotron waves on ions are shown in Figure 9 where the perpendicular ion velocity distributions are shown for three bins at Q_i t=220. The large amplitude density perturbations associated with ion cyclotron waves have penetrated up to the third bin by this time. We therefore expect that the temperature in the first and second bins is more or less heated up to the maximum value determined from the marginal stability analysis (Okuda and Ashour-Abdalla, 1983).
It is very interesting to realize the presence of high energy tail in Figure 9 where the total distribution is separated into bulk and tail parts. The initial Maxwellian distribution is also shown for comparison in the figure. The heated distribution has a high energy tail extending almost as much as 100 times of the initial thermal energy. The temperature of the bulk distribution is about 5-10 times of the initial Maxwellian while that of the tail distribution 50-100 times of the initial temperature.

Figure 9. Ion density profile and the ion perpendicular velocity distribution at four locations at $\Omega_i t = 220$. 
Figure 10 shows similar plots for the electron distribution at $\Omega_1t=175$ for three different bins. It is seen that the electron distribution generally has a plateau at far right such as in bin 4, whereas the distribution tends to have a positive slope for $v_e<v_{de}$ in bins 1 and 2. This suggests that the electron distribution is determined by a delicate balance between wave-induced diffusion and input from the source. Note the plateau formation on the electrons is a subtle process which does not require much energy at all.

![Electron Density Graph](image)

![Parallel Electron Distribution Functions](image)

**Figure 10.** Electron density profile and the electron parallel velocity distribution at three different locations at $\Omega_1t=175$.

4. FORMATION OF AURORAL ARC ELEMENTS

Observations of ion cyclotron waves (Kintner et al., 1979; Yau et al., 1983) and of conic ion distributions on high-latitude field lines (Sharp et al., 1977; Klumpar, 1979; Ungstrup et al., 1979; Gorney et al., 1983) motivated a series of extensive theoretical studies of ion cyclotron turbulence on auroral field lines (Lysak et al., 1981; Papadopoulos et al., 1980; Singh et al., 1981; Dusenbery and Lyons, 1981).
1981: Ashour-Abdalla et al., 1981; Okuda and Ashour-Abdalla, 1983). These theoretical studies focused on ion heating due to the ion cyclotron turbulence and showed that both O+ and H+ ions can be accelerated perpendicular to field lines resulting in enhanced ion fluxes near 90° pitch angle.

In this section we focus on the nonlinear mode-coupling effects of the electrostatic ion cyclotron (EIC) turbulence across the magnetic field. The simulation model is assumed two-dimensional in which the ion cyclotron waves are allowed to propagate in the x-y plane (i.e., k_z=0) in an external uniform magnetic field which is in the y-z plane satisfying B_y>B_z. The ratio B_y/B_z=0.1 is chosen in our simulation model. The electron perpendicular motion is approximated by the guiding center drift in the simulation while the electron parallel motion and the ion dynamics are treated fully without approximation (Lee and Okuda, 1978). The model is initialized by a drifting Maxwellian electron distribution streaming along the external field and a stationary Maxwellian ion distribution. Note that the x-axis is parallel to the north-south direction; the y-axis is parallel to the east-west direction. The tilting of the magnetic field in the y-z plane (with B_y/B_z=0.1) is as approximation of the field (B_y) due to the field-aligned currents (Tajima and Potemra, 1976). The assumed velocity profile is an approximation of the condition of the electron flux being accelerated through the inverted-V potential drop.

Note that our choice of the magnetic field orientation excludes the current-driven instabilities propagating along field lines such as Buneman and ion-acoustic instabilities. Earlier two-dimensional simulations suggested that such instabilities saturate at low level and do not affect the EIC instability appreciably (Pritchett et al., 1981). Furthermore the perpendicular electric fields associated with such instabilities propagating along field lines are small and therefore cannot generate density striations across field lines.

The simulation is performed on a 128x64 grid in the x-y plane with 73,728 electrons and ions. The electron streaming speed is \( V_{do} = 2V_e \) where \( V_e \) is the electron thermal speed. The ratio of the electron gyrofrequency to plasma frequency is \( \omega_{pe}/\omega_{ce} = 5 \) and the time step of integration is \( \omega_{pe} \Delta t = 5 \). The ion to electron mass ratio is \( m_i/m_e = 400 \). The initial ion gyroradius is \( \rho_i = 4 \) grid size. The electron streaming speed is maintained by the recycling scheme (Okuda and Ashour-Abdalla, 1981) with a recycling rate \( \delta = 5 \times 10^{-3} \Delta t \). This recycling scheme is a technique to maintain a flow of the drifting Maxwellian electron distribution along the inverted-V field lines. An electron streaming speed of \( \sim 2V_e \) or greater can be expected to prevail along a large fraction of the acceleration region, and certainly below the acceleration region. It should be noted that the simulation model as described above is strictly valid only in regions where the electrons have been accelerated through at least a fraction of the total potential drop and not too far below the acceleration region where the cold ambient electrons are still a minor constituent.
Figure 11. The number density profile $n_e(x)$ and the equipotential contours at $\Omega_i t = 25$ and 100 in a two-dimensional simulation. Note the development of density striations across magnetic field.

Figure 11 shows the equipotential contours and the electron density $n_e(x)$ averaged over $y$ associated with the ion cyclotron waves. During early stages of the simulation ($\Omega_i T = 25$) the equipotential contours due to the ion cyclotron turbulence exhibit little preferred alignment with little density striations. Note the presence of small scale contours whose sizes are on the order of the initial ion gyroradius. As the simulation develops well into the nonlinear stage ($\Omega_i T = 100$), the equipotential contours and the constant density contours start to striate along the $y$ axis (east-west
direction). The amplitude of the density modulation grows in time and saturates at a maximum variation of \( n_{\text{max}}/n_{\text{min}} = 2 \). Note that the ion gyroradius is several times larger than the initial value due to the perpendicular ion heating by the ion cyclotron turbulence (Okuda and Ashour-Abdalla, 1981).

Variations in the electron streaming speed in our simulations are small compared with variations in the electron number density so that current density striation is produced mainly by the number density striation. It follows that the electron energy flux is also striated in accordance with the electron number density in our simulations. Thus, the intensity of the striations in the field-aligned current and the electron energy flux are both on the order of the number density striation \((n_{\text{max}} - n_{\text{min}})/n_{\text{min}} > 100\% \). It is important to note that fine scale variations of field-aligned current density up to \( -50\% \) of the background current density within an inverted-V scale precipitation region have been measured by sounding rocket experiments conducted by Evans et al. (1977). However, association of these fine scale current density enhancements with auroral arc elements have yet to be established observationally. To recapitulate we emphasize that the striations in number density, field-aligned current and electron energy flux due to ion cyclotron turbulence are the main results of our simulations. The proposed connection between the striations in our simulations and the auroral arc elements is based on plausible arguments rather than observational facts.

The physical mechanism leading to the east-west striations in our simulation can be identified with a nonlinear mode-coupling process between electrostatic ion cyclotron waves. Frequency analysis of wave modes in the simulation reveals that the striation corresponds to a condensation of the wave energy into a zero-frequency d.c. mode (Okuda and Dawson, 1973). Such a condensation phenomenon has been demonstrated in unstable drift waves (Cheng and Okuda, 1978: Sagdeev et al., 1978a) and Alfvén waves (Sadegeev et al., 1978b). On this basis, the striation in our simulation can be interpreted as resulting from nonlinear mode coupling between two ion cyclotron waves having the same \( k_{\parallel} \) but different \( k_{\perp} \) (Cheng and Okuda, 1978: Sagdeev et al., 1978a,b). Since the frequencies of ion cyclotron waves are very close to the ion gyrofrequency when the ion perpendicular temperature is much greater than the ion parallel temperature (Okuda and Ashour-Abdalla, 1981), the nonlinear beating of two ion cyclotron waves with the same \( k_{\parallel} \) can produce a zero-frequency mode with \( k_{\parallel} = 0 \). Once such modes are generated across the magnetic field, they produce quasi-steady state density striations which persist on a time scale much longer than the ion gyroperiod owing to the slow dissipation associated with the ion viscosity (Okuda and Dawson, 1973). Only a slow diffusive process can destroy such d.c. structures. We are aware of the possibility that the condensation of ion cyclotron turbulence into a zero-frequency mode is just one example of a class of nonlinear phenomena which generate quasi-stationary macrostructures from microinstabilities.
5. DISCUSSIONS

We have given an example to show that how to apply particle simulations to a study of ion heating and electron beam propagation in a magnetic field. Only the electrostatic ion cyclotron instabilities have been considered as they are the most relevant instabilities on auroral field lines. It is clear that different boundary conditions will result in very different results of ion heating and beam propagation.

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