REC'D 01 01 01

85003 1985

UCRL-92259
PREPRINT

CONF-850264 - 8

UCRL--92259

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DE85 016088

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This paper was prepared for the proceedings
for the International School for Space Simula-
tions held in Kauai, HI, Feb. 4-15, 1985.

March 3, 1985

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IMPLICIT PLASMA SIMULATION

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ABSTRACT Implicit time integration methods have been used extensively in numerical modelling of slowly varying phenomena in systems that also support rapid variation. Examples include diffusion, hydrodynamics and reaction kinetics. This article discusses implementation of implicit time integration in plasma codes of the "particle-in-cell" family, and the benefits to be gained.

1. INTRODUCTION

In plasmas, many instability, dissipation and nonlinear saturation mechanisms are kinetic in nature, i.e., fluid descriptions are inadequate. The most adaptable and reliable tools for study of complex kinetic plasma behavior are the "particle-in-cell" (PIC) codes, in which the plasma evolution is modeled by 10^3 - 10^7 simulation "particles", each representing a large number of plasma particles, and moving according to the classical Newton-Lorentz equations of motion in fields governed by Maxwell's equations. Characteristic time scales for collective phenomena in plasmas encompass many orders of magnitude. Already applied very successfully to studies of the nonlinear evolution of plasma phenomena on the faster time scales, there is great value in extending PIC techniques to kinetic phenomena on much longer time scales.

One approach to modeling long time-scale behavior in such systems is to alter the governing equations to eliminate uninteresting high frequency modes. Examples, such as Darwin field and hybrid PIC-fluid approximations, are described at this meeting and in chapters in the volume "Multiple Time Scales" in the series *Computational Techniques* (Academic Press, 1985). Here I discuss implicit time integration, which transforms the high-frequency modes into *damped* modes.

The divisions of this article are as follows: The remainder of this Section defines the explicit electrostatic PIC algorithm.

introducing the notation to be used throughout this article, and outlines the properties of explicit differencing and an implicit scheme. Section II presents the "direct" and "moment" implicit methods as applied to the electrostatic field case, along with some results, and discusses remaining limitations on time step, conservation properties, and linear stability theory. In Section IV the direct method is generalized to include the full electromagnetic field.

Langdon and Barnes (1985) provide more detail on all these subjects and others, plus many references.

I.A. Characteristic Time Scales in Weakly-Collisional Plasma

The highest frequencies are associated with the small mass of electrons and the high speed of light. The Langmuir frequency, ω_{pe} , also called simply the plasma frequency, characterizes charge-separation oscillations. Others include the cyclotron frequency, ω_{ce} , and the transit time for electrons or light to cross a characteristic distance.

In contrast, long time scales can be set by ion inertia, electromagnetic effects, and large spatial scale lengths. The ratios of electron to ion plasma and cyclotron frequencies, and of hydrodynamic to electron transit times, are determined by the small number Zm_e/m_i , where Z is the ionic charge state. Where the dominant forces are from magnetic fields due to currents in the plasma itself, the frequencies are reduced relative to ω_{pe} by at least the ratio c/v_e , where c and v_e are light and electron speeds.

I.B. PIC Electrostatic Force Calculation

Originally developed at Stanford, PIC plasma simulation models use a spatial grid to mediate the particle interactions. A charge density is formed from the particle positions onto a spatial grid. Using partial difference equations on this grid, an electric field is found. Then the particles are individually advanced in time using classical equations of motion with the acceleration found by interpolation from the electric field on the grid.

To avoid clutter, we temporarily restrict the discussion to one dimension. At the grid point located at $X_j = j\Delta x$, where Δx is the grid spacing, the charge density ρ_j is formed by adding the contributions of the simulation particles at positions $\{x_i\}$

$$\rho_j = \sum_i q_i S(X_j - x_i) \quad (1.1)$$

where i is the particle index, q_i the charge, and S the particle-grid interpolation spline. Most present work is done with multilinear weighting. In one dimension, S is the linear spline, a tent-shape extending over two cells and zero elsewhere.

From ρ a potential and an electric field are derived on the same mesh. These satisfy relations such as

$$E_j = - \frac{\phi_{j+1} - \phi_{j-1}}{2\Delta x} \quad (1.2)$$

$$\frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2} = -\rho_j \quad (1.3)$$

in rationalized cgs units. Additional smoothing is often applied to ρ_j or ϕ_j .

The particle force field is obtained by an interpolation of the form

$$F_i = q_i \Delta x \sum_j E_j S(X_j - x_i) \quad (1.4)$$

where the sum is over grid points j , and S is the same function used in (1.1).

1.C. Explicit Time Differencing of Particle Equations of Motion

For the integration of the particle equations of motion, numerical time differencing algorithms of the elegant type discussed by Buneman (1967) are almost universally used.

$$\frac{x_{n+1} - x_n}{\Delta t} = v_{n+\frac{1}{2}}; \quad \frac{v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}}}{\Delta t} = a_n + \frac{v_{n+\frac{1}{2}} + v_{n-\frac{1}{2}}}{2} \times \frac{qB_n}{mc} \quad (1.5ab)$$

$$\text{where } a_n = \frac{q}{m} E_n(x_n). \quad (1.5c)$$

and subscript n denotes time level $t_n = n\Delta t$. This is usually called the centered leapfrog scheme.

Equations (1.1)-(1.5) outline the time cycle of an explicit PIC simulation.

In the simplest, unmagnetized case, longitudinal oscillations in a uniform cold plasma consist simply of harmonic oscillations. The properties of the leapfrog scheme are illustrated by considering a single particle with a linear restoring force, $a_n = -\omega_0^2 x_n$, with no magnetic field term. Setting $x_n = X \exp(-i\omega n\Delta t)$, we find for $\omega_0\Delta t < 2$ that ω is real; the oscillations are neither growing nor damped. For $\omega_0\Delta t > 2$, one root has $\text{Im } \omega > 0$; this numerical instability arises for any explicit scheme for $\omega_0\Delta t$ above some threshold of order unity (Cohen *et al.*, 1982). Instability can be avoided through the use of implicit time integration, at the expense of increased complexity.

1.D. Implicit Time Differencing of the Particle Equations of Motion

The first major issue is the choice of finite-differenced equations of motion for the particles that have the necessary stability at large time-step and are accurate enough for the low frequency phenomena to be simulated. We choose not to consider backward-biased schemes with relative errors of order Δt ; it is not expensive to achieve relative error of order Δt^2 , with error $\propto \Delta t^3$ in $\text{Im } \omega$, the growth/decay rate.

Several suitable schemes for time-differencing the particles have been analyzed and applied. Here, we discuss only the "D₁" scheme (Cohen *et al.*, 1982), also called the $\bar{1}$ scheme (Barnes *et al.*, 1983), which can be written

$$\frac{x_{n+1} - x_n}{\Delta t} = v_{n+\frac{1}{2}}; \quad \frac{v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}}}{\Delta t} = \bar{a}_n + \frac{v_{n+\frac{1}{2}} + v_{n-\frac{1}{2}}}{2} \times \frac{qB_n}{mc} \quad (1.6a)$$

$$\text{where } \bar{a}_n = \frac{1}{2}[\bar{a}_{n-1} + \frac{q}{m}E_{n+1}(x_{n+1})]. \quad (1.7)$$

To check the accuracy of this scheme, we can again derive and solve a dispersion relation for harmonic oscillations. For $\omega_0\Delta t \leq 1$, we find (Cohen *et al.*, 1982) $\pm \text{Re } \omega/\omega_0 = 1 - (11/24)(\omega_0\Delta t)^2 + \dots$, $\text{Im } \omega/\omega_0 = -(\omega_0\Delta t)^3/2 + \dots$, and an extraneous damped mode with $|z| \rightarrow \frac{1}{2}$. For $\omega_0\Delta t \gg 1$, all modes are heavily damped, $|z| \sim (\omega_0\Delta t)^{-2/3}$.

Equation (1.6b) can be solved exactly for $v_{n+\frac{1}{2}}$ by adding $\frac{1}{2}\bar{a}_n\Delta t$ to $v_{n-\frac{1}{2}}$, doing a rotation, and again adding $\frac{1}{2}\bar{a}_n\Delta t$. The result is

$$\mathbf{v}_{n+\frac{1}{2}} = \frac{1}{2}\bar{\mathbf{a}}_n\Delta t + R \cdot [\mathbf{v}_{n-\frac{1}{2}} + \frac{1}{2}\bar{\mathbf{a}}_n\Delta t] \quad (1.8)$$

where the operator R effects a rotation through angle $-2\tan^{-1}(\Omega\Delta t/2)$ (where $\Omega \equiv qB_n/mc$).

With explicit differencing, the time-cycle is split between advancing particles and fields; these calculations alternate and proceed independently. A price we pay for implicit differencing is that time-cycle splitting is more complicated. An implicit code must solve the coupled set of equations (1.1)-(1.4), with (1.6-1.7).

II. DIRECT METHOD WITH ELECTROSTATIC FIELDS

In all implicit schemes the future positions $\mathbf{x}_{n+1}$ depend on the accelerations $\mathbf{a}_{n+1}$ due to the electric field $\mathbf{E}_{n+1}$. But this field is not yet known, because it depends on the density ρ_{n+1} of particle positions $\{\mathbf{x}_{n+1}\}$. The solution of this large system of nonlinear, coupled particle and field equations is the other major implementation issue.

II.A. Solution of the Implicit Equations

In the first method implemented for this solution, the fields at the new time level are predicted by solving coupled field and fluid equations. After the fields are known, the particles are advanced to the new time-level. This approach, described in detail by Denavit (1981) and Mason (1981a), is outlined later in this article.

It is also practical to predict the future electric field $\mathbf{E}_{n+1}$ quite directly by means of a linearization of the particle-field equations. Langdon, Cohen and Friedman (1983) and Langdon and Barnes (1985), together with references they cite, cover the work published on the direct method up to early 1984.

1. Outline of the "direct method"

The essence of the "direct" method is that we work *directly* with the particle equations of motion and the particle/field coupling equations. These are linearized about an estimate (extrapolation) for their values at the new time level $n+1$. The future values of $\{\mathbf{x}, \mathbf{v}\}$ are divided into two parts:

- increments $\{\delta\mathbf{x}, \delta\mathbf{v}\}$ which depend on the (unknown) fields at the future time level $n+1$, and
- extrapolations $\{\tilde{\mathbf{x}}_{n+1}, \tilde{\mathbf{v}}_{n+\frac{1}{2}}\}$ which incorporate *all* other contributions to the equation of motion.

The charge density $\tilde{\rho}_{n+1}$, corresponding to positions $\{\tilde{x}_{n+1}\}$, is collected, as are the coefficients in an expression for the difference $\delta\rho(\{E\}) = \rho_{n+1} - \tilde{\rho}_{n+1}$ between the densities obtained after integration with $E = 0$ and with the corrected field E_{n+1} . These comprise the source term in Gauss's law:

$$\nabla \cdot E_{n+1} = \delta\rho(\{E\}) + \tilde{\rho}_{n+1} \quad (11.1)$$

This becomes a linear elliptic equation for ϕ_{n+1} , with non-constant coefficients.

2. A one-dimensional realization

The direct implicit method is illustrated in the following one-dimensional, unmagnetized, electrostatic example. The position x_{n+1} of a particle at time level t_{n+1} , as given by an implicit time integration scheme, can be written as

$$x_{n+1} = \beta \Delta t^2 a_{n+1} + \tilde{x}_{n+1}, \quad (11.2)$$

where $\beta > 0$ is a parameter controlling implicitness and is equal to $\frac{1}{2}$ for the D_1 scheme; $\tilde{x}_{n+1}$, the position obtained from the equation of motion with the acceleration a_{n+1} omitted, is known in terms of positions, velocities and accelerations at times t_n and earlier. Eliminating $v_{n+\frac{1}{2}}$ between (1.6) and (1.7), we find

$$\tilde{x}_{n+1} = x_n + v_{n-\frac{1}{2}} \Delta t + \frac{1}{2} \bar{a}_{n-1} \Delta t^2 \quad (11.3)$$

The charge density $\tilde{\rho}_{j,n+1}$ is formed as in (1.1) by adding the contribution of the simulation particles at positions $\{\tilde{x}_{i,n+1}\}$.

$$\tilde{\rho}_{j,n+1} = \sum_i q_i S(X_j - \tilde{x}_{i,n+1}) \quad (11.4)$$

If we expand S in (1.1) with respect to position, then

$$\delta\rho_{j,n+1} = - \sum_i q_i \delta x_i S'(X_j - \tilde{x}_{i,n+1}) \quad (11.5)$$

with $\delta x_i = x_{i,n+1} - \tilde{x}_{i,n+1}$ and $S'(X) = dS/dX$. In terms of E_{n+1} , the particle acceleration is obtained from (1.4) evaluated at $\tilde{x}_{n+1}$.

$$m_i a_{i,n+1} = q_i \Delta x \sum_j E_{j,n+1} S(X_j - \tilde{x}_{i,n+1}) \quad (11.6)$$

Using (11.6) to express δx in (11.5) provides a "strict" interpretation of the direct method. The care with which we express the increment $\{\delta\rho\}$

is a compromise between complexity, robust behavior, and strong convergence (Langdon *et al.*, 1983; Barnes *et al.*, 1983; Langdon and Barnes, 1985). Here we discuss only the simpler implementations.

Writing (11.5) as

$$\delta\rho = - \left[\nabla \cdot \sum q \delta x S(x - \tilde{x}_{n+1}) \right]_{x=x_j}, \quad (11.7)$$

we see that (11.5) is a finite element representations of

$$\delta\rho = - \nabla \cdot [\tilde{\rho} \delta x], \quad (11.8)$$

With (11.1) we are lead to the elliptic partial difference equation

$$\nabla \cdot [1 + \chi] \cdot \nabla \phi_{n+1} = - \tilde{\rho}_{n+1} \quad (11.9)$$

where $\chi(x) = \beta \tilde{\rho}(x)(q/m)\Delta t^2$ summed over species, i.e. $\chi = \beta(\omega_p \Delta t)^2$. Equation (11.9) is an elliptic field equation whose coefficients depend directly on particle data accumulated on the spatial grid. Because of the similarity of (11.9) to the field equation in dielectric media, we call χ the implicit susceptibility. Where $\omega_p \Delta t$ is large, the regime we wish to access, note that $\chi \gg 1$ is dominant in the right-hand-side of (11.9).

With the extrapolated charge density $\tilde{\rho}_{j,n+1}$ and a reasonable finite-difference representation of the linearized implicit contribution $\delta\rho = - \partial(\chi E)/\partial x$, the field equation in one dimension is

$$\tilde{\rho}_{j,n+1} = \left[(1 + \chi_{j+\frac{1}{2}}) E_{j+\frac{1}{2},n+1} - (1 + \chi_{j-\frac{1}{2}}) E_{j-\frac{1}{2},n+1} \right] / \Delta x. \quad (11.10)$$

Two representation of $\chi_{j+\frac{1}{2}}$ used here are (Langdon *et al.*, 1983, Eqs. (28ab))

$$\chi_{j+\frac{1}{2}} = \frac{1}{2} [\chi_j + \chi_{j+1}] \quad (11.11a)$$

$$\text{or } \chi_{j+\frac{1}{2}} = \max(\chi_j, \chi_{j+1}), \quad (11.11b)$$

$$\text{where } \chi_j = \Delta t^2 \sum_s \left[\beta \tilde{\rho}_{j,n+1} \frac{q}{m} \right]_s \quad (11.12)$$

is a sum over species index s . In both (11.10) and (11.12), $\tilde{\rho}_{j,n+1}$ (for each species differing in q/m) is given by (11.4).

In terms of the field

$$E_{j,n+1} = \frac{1}{2} [E_{j-\frac{1}{2},n+1} + E_{j+\frac{1}{2},n+1}] \quad (11.13)$$

formed from E at half-integer positions, the particle acceleration is evaluated at $\tilde{x}_{n+1}$ using (11.6). This algorithm is the shortest implicit PIC scheme we have seen, and was the most robust in the expansion test problem reported by Langdon and Barnes (1985).

3. General electrostatic case

We return to the multidimensional case, possibly including a magnetic field imposed by external currents. We have

$$\delta x_{n+1} = \delta v_{n+1} \Delta t = T \cdot \frac{q \Delta t^2}{2m} E_{n+1}(\tilde{x}_{n+1}), \quad (11.14)$$

where $T = \frac{1}{2}[I + R_n(\tilde{x}_{n+1})]$, which follows from (1.8).

The implicit term $\delta \rho = -\nabla \cdot (\rho \delta \tilde{x}_{n+1})$ is seen to be

$$\delta \rho = -\nabla \cdot (\tilde{\rho}_{n+1} \delta x) = -\nabla \cdot (\chi \cdot E) \quad (11.15)$$

The implicit susceptibility

$$\chi = \left[\sum_s \frac{\tilde{\rho}_{n+1,s} q_s \Delta t^2}{2m_s} T_s \right] \quad (11.16)$$

is a tensor due to the rotation R induced by B . The [...] is a sum over species s , not each particle. If only the electrons are implicit, only they appear in (11.16). In this case, the terms [...] require only a knowledge of the electrons' ρ [in addition to the net ρ used on the right side of (11.17)]. In general, it is sufficient to accumulate $\tilde{\rho}_{n+1,s}$ separately from species with differing q/m . This requires more storage, but no more computation than for an explicit code.

We now have everything needed to write an equation for $E = -\nabla \phi$. On substituting our expressions for $\tilde{\rho}_{n+1}$ and $\delta \rho$ into the field equation (11.1) we again have the elliptic equation (11.9), except that χ has become a tensor.

If spatial smoothing, denoted by the operator $\hat{S}$, is to be applied to ρ and ϕ on the grid, then $\hat{S}$ must be included in χ if the field solution is to take this into account. In some applications, this has been essential (Sections 11.B.2 and 11.B.3; Barnes *et al.*, 1983). Inconsistent smoothing has consequences to linear stability (Section 11.C.4).

Advancing the Particles

The field E_{n+1} is evaluated at positions $\{\tilde{x}_{n+1}\}$ in (1.4) in integrating the particles to their final positions $\{x_{n+1}\}$. The error resulting from this approximation, and from the linearization of $\delta\rho$, introduces a possible limitation on Δt that depends on field and density gradients; see section 11.C.1.

After advancing each particle to position x_{n+1} , one can immediately calculate its $\tilde{x}_{n+2}$ and its contribution to $\tilde{\rho}_{n+2}$. In this way, only one pass through the particle list is required per time step, an advantage when the particles are stored on slower memory devices, such as rotating magnetic disk.

4. The "Moment" Implicit Method

The "moment implicit" method uses velocity moment equations to predict ρ in terms of the future E . The moment equations are closed by accumulating flux and stress tensor moments from the particles at the *known* time level.

$$J_{n+\frac{1}{2}} = J_{n-\frac{1}{2}} - \frac{q\Delta t}{m} \left[\frac{\partial P_n}{\partial x} - \rho_n E_{n+1} \right] \quad \text{-backward Euler}$$

$$\frac{\partial}{\partial x} E_{n+1} = \rho_{n+1} \approx \rho_n - \Delta t \frac{\partial}{\partial x} J_{n+\frac{1}{2}}$$

where $(\rho, J, P) = n(q, qv, mvv)$ are formed as sums over known particle coordinates. Eliminating $J_{n+\frac{1}{2}}$,

$$\frac{\partial}{\partial x} E_{n+1} = \rho_n - \Delta t \frac{\partial}{\partial x} \left[J_{n-\frac{1}{2}} - \frac{q\Delta t}{m} \frac{\partial P_n}{\partial x} \right] - \frac{q}{m} \Delta t^2 \frac{\partial}{\partial x} (\rho_n E_{n+1})$$

This equation is solved for E_{n+1} , with which the particles are integrated.

The field predictor (11.9) has some features in common with the field predictor in the moment method. This is not surprising since both methods attempt an approximate solution of similar equations. The relation of terms arising in the implicit moment and direct implicit viewpoints is discussed by Mason (1985) and Langdon *et al* (1983); here we summarize. The equation for E_{n+1} can be rewritten as

$$\frac{\partial}{\partial x} E_{n+1} = \tilde{\rho}_{n+1} - \frac{\partial}{\partial x} (\chi_n E_{n+1})$$

where we have expressed the moment-method terms using symbols from the direct method. The counterpart to χ in the moment method is approximated from the density ρ_n rather than being formed from $\tilde{\rho}_{n+1}$. The source term $\tilde{\rho}_{n+1}$ is replaced by ρ_n plus the divergence of current and stress tensor terms.

$$\tilde{\rho}_{n+1} \approx \rho_n - \Delta t \frac{\partial}{\partial x} \left[J_{n-\frac{1}{2}} - \frac{q \Delta t}{m} \frac{\partial P_n}{\partial x} \right]$$

If there could be no finite-difference errors, this combination would equal $\tilde{\rho}_{n+1}$. These approximations result in a stability constraint $k v_i \Delta t \lesssim 1$ or $k v \Delta t \lesssim 1$ (Section 11.C.1) that does not arise in the direct method, as well as requiring more computation.

Insight gained from the direct method shows how to eliminate the stress tensor, which contributes to the $k v_i \Delta t$ constraint in moment codes (Brackbill and Forslund, 1985; Wallace *et al.*, 1984). Experience with moment codes using ad hoc spatial differencing encouraged experimentation with simpler differencing in direct codes. As moment and direct codes are borrowing features from each other, the distinction becomes more one of viewpoint in deriving algorithms and less in the resulting codes themselves. Design of optimal codes requires understanding the fruits of both viewpoints.

11.B. Demonstrative results

1. Free expansion of a plasma slab

Denavit (1981) used the one-dimensional expansion of a plasma slab as a check on his early moment-method code. Featuring sharp gradients initially and a large range of densities, this problem is also used to check and improve variations of direct-method algorithms. Langdon *et al.* (1984), as outlined here, sought to isolate those forms most suitable for extension to a two-dimensional and electromagnetic code. Without resort to spatial smoothing, adequate accuracy and robust behavior were obtained. With $n \Delta x = 64$ particles per cell in the slab initially, and values of $\omega_{pe} \Delta t$ as large as 120 (much larger than have been reported previously for unmagnetized plasma), they find that two parameters measure the stress on the algorithm. One parameter is $v_i \Delta t / \Delta x$, the ratio of thermal electron transit distance per cycle to the zone size. With $v_i \Delta t / \Delta x > 1$, energy conservation is degraded in the absence of spatial smoothing.

The more important parameter is $\chi_1 = \beta q^2 \Delta t^2 / m |\Delta x|$, where q and m are the particle charge and mass, and $|\Delta x|$ the zone volume. This is a worst-case measure of the validity of linearization in the field prediction, as stressed by short-wavelength sampling fluctuations in the charge density. Using the algorithm of Section 11.A.2 with either (11.11a) or (11.11b), they obtain reasonable results with χ_1 well over 100. Most other variants suffer nonlinear numerical instability at the edge of the expansion when $\chi_1 \gtrsim 1$.

With χ_1 written as $\beta (\omega_{pe} \Delta t)^2 / N_c$, where N_c is the number of particles per cell ($n \Delta x$ in one dimension), the value of being able to run with $\chi_1 \gg 1$ is clarified. Many applications of two-dimensional explicit codes require only $N_c \gtrsim 10$. If we were restricted to $\chi_1 \lesssim 1$, we would need a number of particles per cell exceeding $(\omega_{pe} \Delta t)^2$, which would be a severe limitation.

2. Ion-acoustic fluctuations of a nonequilibrium plasma

Ion-acoustic fluctuations of a uniform, thermal, unmagnetized, two-temperature, one-dimensional plasma are examined by Barnes *et al.* (1983). Since the ion-acoustic fluctuations represent an extremely small part of the total fluctuation energy of a thermal plasma and are strongly affected by electron Landau damping in the parameter range studied, these results represent a severe test of the applicability of the model.

The time step was fixed at $\omega_{pe} \Delta t = 10$, a factor of 50-100 over that possible for an explicit algorithm. The fluctuation spectra are compared for the cases in which the resonant electron response is retained by the direct implicit method, and in which the low-frequency electron response is only adiabatic. The ratio of the former to the latter is approximately T_e/T_i , which is 20 in the example. The fluctuation spectrum in the simulation indicates that the resonant electron response at low frequencies is described accurately by the implicit method. Also, fluctuations at mode frequencies higher than the ion-acoustic range have been suppressed.

3. Gravitational interchange instability of a magnetized plasma

Using the direct method, and treating both the electrons and ions as zero gyroradius particles, an unstable gravitational interchange is studied for an inhomogeneous two-dimensional magnetized plasma (Barnes *et al.*, 1983).

The effect of the polarization motion of the ions is very important for this high-density plasma ($\omega_{pi}/\Omega_i \gg 1$). If the polarization motion is

neglected, the growth rate becomes unphysically large for high density. For the simulation parameters considered here, the physical growth rate is 1/7 the growth rate found neglecting polarization. In the simulation, an extremely large time step of $\omega_{pe}\Delta t = 10^3$ was used. The observed growth rate is within 15% of the theoretically predicted value, verifying the correct modeling of ion polarization motion.

11.C. Properties of Implicit Particle Codes

1. Remaining limitations on time step

Although we have largely overcome the stability limit on $\omega_{pe}\Delta t$, there remain restrictions that involve Δt . In addition to the aspects discussed under the following subheadings, Sections 11.C.3 and 11.C.4 are also relevant.

Doppler frequency limit

When a particle moves in one time step a distance greater than a scale length L for spatial variation of fields, the particle does not sample the field sufficiently closely in space to respond accurately to the field structure. In analysis, this is stated in terms of the Doppler-shifted frequency $\omega - k \cdot v$. If the thermal spread of electron velocities $v_t = (T_e/m_e)^{1/2}$, and wavenumber k are such that $kv_t\Delta t \geq 1$, then the Doppler-shifted frequency exceeds Δt^{-1} for a large fraction of the electrons. It is not surprising that the collective response is qualitatively incorrect, showing an excess of shielding, as indicated by the dielectric function becoming

$$\epsilon \approx 1 + \beta\omega_{pe}\Delta t^2 + (\text{ion response})$$

instead of the correct result,

$$\epsilon \approx 1 + (k\lambda_D)^{-2} + (\text{ion response})$$

Violation of the restriction $kv_t\Delta t \lesssim 1$ in direct-method electrostatic codes does not, in general, result in instability. In many applications, the sharp field gradients may arise only during time intervals or in spatial regions such that the inaccuracy does not interfere with the purpose of the simulation. In contrast, strong instability observed with the moment method has been traced to a constraint on $kv_t\Delta t$ (Sakagami *et al.*, 1981; Denavit, private communication) and is attributed to lack of convergence (Denavit, 1981; Cohen *et al.*, 1982a). Such instability, as opposed to innocuous inaccuracy, is disruptive to the simulation. The ability of a direct-implicit code to remain stable is useful with nonuniform meshes

where some cell dimensions may be much smaller, and helps evade failures due to uninteresting transients or small regions.

The Doppler frequency, or transit time, limit is analyzed by Denavit (1981), Cohen *et al* (1982), Langdon *et al* (1983), Langdon and Barnes (1985), and references therein.

Limits due to field and density gradients

Linearization of the time-advanced charge density breaks down when field or density gradients are too large. Nonetheless, the codes have been made to function successfully (Section 11.B.1), but convergence is not guaranteed.

Evaluation of δx in terms of E_{n+1} at $\tilde{x}_{n+1}$ rather than at x_{n+1} creates an error $\approx \delta x \cdot \nabla E$. Denavit (1981) interprets this term in terms of the frequency of oscillation of a particle trapped in a local potential minimum. The relative error is $\beta(\omega_{\text{trap}} \Delta t)^2$. To compare the severity of this and the transit-time limitations, note that

$$\beta(\omega_{\text{trap}} \Delta t)^2 = \beta(kv_e \Delta t)^2 q\phi/T_e$$

Thus, if we take $kv_e \Delta t \lesssim 1$ as given, the linearization is justified if $q\phi \lesssim T_e$. Put another way, if $kv_e \Delta t \lesssim 1$, then $(\omega_{\text{trap}} \Delta t)^2 = ka\Delta t^2$ is small if $a\Delta t$, the impulse in one time step, is small compared to v . In grossly nonneutral regions, where the net charge $\Delta\rho$ is comparable to the electron charge ρ_e ,

$$\beta(\omega_{\text{trap}} \Delta t)^2 \approx (\omega_{pe} \Delta t)^2 \Delta\rho/\rho_e$$

will not be small unless $\omega_{pe} \Delta t$ is small in that region.

The expression $\delta\rho = -\nabla \cdot (\rho \delta x)$ is valid when δx is smaller than density gradient scale lengths.

The validity of linearization is treated by Denavit (1981), Langdon *et al* (1983), Cohen *et al* (1984), Langdon and Barnes (1985), and references therein.

3. Energy Conservation and Artificial Cooling

To understand better the origins and control of nonphysical cooling [a manifestation of error in codes using damped equations of motion (Adam *et al.*, 1982; Barnes *et al.*, 1983)], the Lenard-Balescu collision operator corresponding to implicit time integration is examined by Langdon and Barnes (1985), based on the kinetic theory in Birdsall and Langdon (1985), Chapters 9 and 12. They find two spurious terms due to phase errors associated with damping. One is a nonresonant contribution to the polarization drag. That is, the Cerenkov wake of plasmons, excited by the passage of a particle, is nonphysically damped. The other term is a spurious nonresonant contribution to dynamical friction and corresponds to the drag calculated by Cohen *et al.* (1982) but with the field given by the thermal fluctuation spectrum.

Quantitative calculations of cooling rates based on the kinetic theory have not yet been carried out. However, cooling rates observed in simulations of thermal plasmas (Barnes, *et al.*, 1983) indicate that cooling is likely to be dominated by damping of a broad band of thermal fluctuations. Thus, the reduction in cooling for schemes with third-order damping compared with those with first-order damping is much less than the reduction in the damping of low-frequency plasma modes. Further, the most effective means of reducing cooling is to cut the width of the fluctuation spectrum by cutting off in wavenumber (spatial smoothing) or in frequency (by increasing Δt).

4. Effects of imperfect field solution on linear stability and dispersion

In practice, because simplifications are used in the representation of the $\nabla \cdot \chi \cdot \nabla \phi$ term, and iteration is not used in practice, the intended equations, (1.1)-(1.4) and (1.6)-(1.7), are not actually satisfied by the code. Analysis of linear stability and dispersion in uniform plasma, as described by dispersion relations that take into account the actual space and time difference methods, provides guidance to behavior to be expected. In particular, the consequences of various simplifications of the field equation operator have been analyzed by Cohen *et al.* (1984), and by Langdon and Barnes (1985).

II.D Generalizations

Many generalizations are possible. "Gyro-averaged particle simulation" (GAPS) removes the cyclotron frequency while retaining finite-Larmor-radius effects. Combinations of fluid and implicit particle descriptions have been made by Mason (1981, 1985) and Denavit (1983, and this meeting). If a component of the plasma is modeled by fluid equations then those equations are linearized to find $\{\delta\rho, \delta J\}$ (Denavit, 1983).

III. ELECTROMAGNETIC DIRECT IMPLICIT METHOD

Until recently, most plasma simulation including the full electromagnetic field was done with explicit differencing of both the particles and fields. The latter adds a Courant-Levy-Friedrichs time-step limitation $\Delta t < c/\lambda$, where λ is approximately the mesh spacing used for the fields. This limitation has been removed in two ways. One is to alter the field equations so that they no longer support wave propagation. A proven approach here is the Darwin, or magnetoinductive, model. Another is to use implicit differencing of the field equations. Recently, codes have used implicit differencing of both fields and particles.

Darwin codes (Hewett, this meeting) eliminate the Courant restriction $\Delta t < c/\lambda$ by dropping Maxwell's transverse displacement current term. These "pre-Maxwell equations" eliminate electromagnetic wave propagation while retaining electrostatic, magnetostatic, and inductive electric fields. Nielson and Lewis (1976) provide many references for the historical development of these codes. For applications not requiring a kinetic description of the electrons, codes using a hybrid of particle ions and fluid electrons are indicated. With Darwin and quasistatic approximations, long time scales are accessible, as in a fully implicit code, but with less noise (Hewett, 1980, and references therein).

Implicit fields reproduce electromagnetic wave propagation at long wavelengths ($\gg c\Delta t$). At short wavelengths, the electrostatic, magnetostatic, and inductive electric fields are retained, as in a Darwin code. Implicit fields can be used with explicit particles. With implicit particles, Langmuir waves are stabilized at all wavelengths, as in an implicit electrostatic code. The electrostatic fields are accurate for wavelengths longer than the electron transit distance ($v_{te}\Delta t$). These properties make an implicit electromagnetic code attractive, e.g., to modeling of reconnection and of intense particle currents.

Here we outline a fully implicit electromagnetic algorithm that has been implemented by Hewett and Langdon. Barnes and his co-workers have another version of this algorithm. Brackbill and Forslund (1985) and Mason (1985) describe moment method electromagnetic algorithms. Wallace, Brackbill and Forslund (1985) describe an algorithm that incorporates aspects of both viewpoints.

III.B Implicit Electromagnetic Fields

Here we must select a time-differencing scheme for the fields, and find a method for solving the coupled field and particle equations. The Maxwell equations in rationalized cgs units are time-differenced using the D_1 implicit scheme as

$$c\nabla \times B_{n+\frac{1}{2}} = J_{n+\frac{1}{2}} + \frac{E_{n+1} - E_n}{\Delta t} \quad (III.1a)$$

$$-c\nabla \times \bar{E}_n = \frac{B_{n+\frac{1}{2}} - B_{n-\frac{1}{2}}}{\Delta t} \quad (III.1b)$$

$$\text{where } \bar{E}_n = \frac{1}{2}[E_{n-1} + E_{n+1}] \quad (III.1c)$$

is the result of a recursive low-pass filter with phase error $O(\Delta t^3)$. This phase error is an advance, not a lag as one gets if E_{n+1} is not used, so it provides dissipation of inaccurately calculated short wavelengths, in particular, stability when $c\Delta t \gg \Delta x$. In the limit $ck\Delta t \gg 1$ the fields are close to those in the Darwin approximation. Long wavelengths are weakly damped, $\text{Im } \omega(k)/ck = -\frac{1}{2}(ck\Delta t)^3$.

To form a B_n for use in the particle mover, we use, e.g.

$$B_n = B_{n-\frac{1}{2}} - \frac{1}{2}\Delta t \, c\nabla \times E_n \quad (III.2)$$

We use E_n , rather than $\bar{E}_n$ as in (III.1b), to simplify the linearized particle equation.

III.C The Direct Method for Implicit Particles and Fields

As in Section II.A.3 for the electrostatic case, the source terms in Maxwell's equations (III.1) are the densities $\{\tilde{\rho}_{n+\frac{1}{2}}, \tilde{J}_{n+\frac{1}{2}}\}$ and $\{\delta\rho, \delta J\}$ corresponding to the extrapolations $\{\tilde{x}_{n+1}, \tilde{v}_{n+\frac{1}{2}}\}$, plus the increments $\{\delta x, \delta v\}$ that depend on E_{n+1} .

The extrapolated current and charge densities $\{\tilde{\rho}_{n+\frac{1}{2}}, \tilde{J}_{n+\frac{1}{2}}\}$ are evaluated as in explicit codes, such as ZOHAR (Langdon and Lasinski).

1976) and the Los Alamos WAVE code, from $\tilde{x}_{n+1}$, $\tilde{v}_{n+1/2}$ and x_n . At the grid point located at X_j , $\tilde{\rho}_{n+1}$ is given by (II.4),

$$\text{and } \tilde{J}_{n+1/2} = \sum q \tilde{v}_{n+1/2} S(X_j - \frac{1}{2}[x_n + \tilde{x}_{n+1}]) \quad (\text{III.3a})$$

$$\text{or } = \sum q \tilde{v}_{n+1/2} \frac{1}{2}[S(X_j - x_n) + S(X_j - \tilde{x}_{n+1})] \quad (\text{III.3b})$$

Consistency of $\tilde{J}_{n+1/2}$ and $\tilde{\rho}_{n+1}$ with the finite-differenced continuity equation is ensured by a correction to the longitudinal component of $\tilde{J}$ or of E_{n+1} (Langdon and Birdsall, 1985, and references therein). Here, we replace $\tilde{J}_{n+1/2}$ with $J'_{n+1/2} = \tilde{J}_{n+1/2} + (\nabla \psi)/\Delta t$. Langdon and Barnes (1985) discuss solution for ψ , and an alternate correction to E_{n+1} .

As in deriving the expression for $\delta\rho$, Eq. (II.8), δJ can be shown, by linearization of the expression for $J_{n+1/2} - \tilde{J}_{n+1/2}$, to be of the form

$$\delta J = \rho \delta v - \frac{1}{2} \nabla \times (J \times \delta x) \quad (\text{III.4})$$

for each species, where superscript ($\sim$) is understood for ρ and J on the right side. Langdon and Barnes (1985) give a heuristic derivation of (III.4). The second term is needed, e.g., to retain Galilean invariance. With (II.14) and (II.15), we write the implicit terms as $\tilde{\rho}_{n+1} \delta v = \chi \cdot E_{n+1} / \Delta t$ and $\tilde{J}_{n+1/2} \times \delta x = c \xi \cdot E_{n+1}$, where ξ is a tensor given by a sum over species γ .

We now have everything needed to write an equation for E_{n+1} . On substituting our expressions for $\tilde{J}_{n+1/2}$ and δJ into the field equations (III.1), we have

$$c \Delta t \nabla \times [B_{n+1/2} + \frac{1}{2} \xi \cdot E_{n+1}] = J'_{n+1/2} \Delta t + \chi \cdot E_{n+1} + (E_{n+1} - E_n) \quad (\text{III.5a})$$

$$- \frac{1}{2} c \Delta t \nabla \times [\bar{E}_{n-1} + E_{n+1}] = B_{n+1/2} - B_{n-1/2} \quad (\text{III.5b})$$

the divergence of the Ampere-Maxwell equation (III.5a) recovers our electrostatic implicit field equation, (II.9) with $E_{n+1} = -\nabla \phi_{n+1}$.

III.D Applications of Implicit Electromagnetic Codes

For my interests, implicit methods will be most profitable in electromagnetic and hybrid codes. Applications have been made at Los Alamos to electron transport (Forslund and Brackbill, 1982; Mason, 1985), Weibel instability (Brackbill and Forslund, 1982), lower hybrid drift instability (Brackbill *et al.*, 1984), and space plasma problems (Quest *et al.*, 1983; Forslund *et al.*, 1984). Preliminary results from direct-method electromagnetic codes have been obtained by D. Barnes and his co-workers at IFS and Nagoya, and by Hewett and Langdon (1985).

ACKNOWLEDGMENTS

This article is mainly a summary of Langdon and Barnes (1985). This work was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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