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IMPLICIT METHODS IN PARTICLE SIMULATION

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Abstract

This paper surveys recent advances in the application of implicit integration schemes to particle simulation of plasmas. The use of implicit integration schemes is motivated by the goal of efficiently studying low-frequency plasma phenomena using a large timestep, while retaining accuracy and kinetics. Implicit schemes achieve numerical stability and provide selective damping of unwanted high-frequency waves. This paper reviews the implicit moment and direct implicit methods. Lastly, the merging of implicit methods with orbit averaging can result in additional computational savings.

I. Introduction

Particle codes are the most versatile and reliable tools for the study of complex kinetic plasma behavior. These codes follow the trajectories of thousands of sample particles in electromagnetic fields calculated self-consistently from Maxwell's equations. The numerical stability of these codes previously required resolution of the fast time scales associated with high-frequency waves. This was a significant limitation when the phenomena of interest occurred on much longer time scales. The recent introduction of implicit time integration schemes[1,2,3] has partially removed these restrictions.

It has long been recognized that implicit time integration was needed to relax timestep constraints in particle codes.[4,5] The major inhibition has been the very large number of nonlinear equations to be solved simultaneously. In the last two years a number of researchers[1,2,3] independently formulated implicit particle codes. They exhibited the dependence of the plasma response (the charge and current densities ρ and $\vec{J}$) on the electric field, linearized, and obtained a sparse matrix equation of rank equal to the number of electric and magnetic field quantities defined on the spatial grid. Solution was then achieved by standard methods.

Currently there are two principal approaches to implicit particle simulation. Mason[1] and Denavit[2] introduced fluid moment equations describing charge and momentum conservation as intermediaries between the particle and field equations. Brackbill and Forslund[6] extended this method to two-dimensional electromagnetic simulation. The implicit moment equation approach (Sec. II) can be viewed as a kinetic extension of a class of fluid-particle hybrid simulation techniques in which a fluid species is advanced implicitly.[7,8]

A more direct implicit approach (Sec. III) has been introduced and refined by Friedman, Langdon, and Cohen,[3,9] in which no auxiliary equations are introduced. In an electrostatic model, the charge density at the advanced time level is linearized about an explicit approximate density: and an increment is computed that is linear in the advanced field. The resulting field equation is elliptic, with coefficients depending on particle data accumulated on the spatial grid in the form of a susceptibility. The particles are advanced serially in a conventional manner. The direct implicit particle method has been formulated in two dimensions[9] and for electromagnetic simulation.

Another class of methods that improves particle code efficiency takes advantage of multiple time scales (Sec. IV). In an orbit-averaged magneto-inductive algorithm,[10] particles are advanced with a small timestep to resolve their orbits. An explicit solution for the fields, omitting electrostatic fields, is obtained using currents accumulated from the particles and temporally averaged. This reduces the number of particles and permits a large timestep for the field advance. Orbit averaging in an electrostatic model requires an implicit field solution if a long timestep is desired.[11] In an explicit algorithm using electron subcycling,[12] ions are advanced with a large timestep much less often than the electrons are advanced and Poisson's equation is solved, making the cost of the ions negligible. Application of the gyrokinetic formalism employing analytical gyrophase averaging has also extended explicit codes to longer timesteps.[13]

An overview of design criteria, limitations, and future research directions is presented in Sec. V.

II. Hybrid Simulation Models and Implicit Moment Equations

Hybrid Models. Implicit time integration schemes have been applied to models in which fluid equations are used to represent one species and a particle description is taken for another. Two representative models are now being used to study magnetically confined plasmas that exhibit strong diamagnetic effects.[7,8]

Hewett[7] has formulated a two-dimensional (r-z) hybrid simulation code to study magnetic pinches, whereas Cohen and Brengle[8] have performed one-dimensional (r) hybrid simulations of (magnetic) field-reversed plasmas. In both schemes, ions are simulated as particles and advanced explicitly; the electrons are an inertialess fluid with equation of motion,

$$0 = -\vec{E} - \frac{\nabla n_e T_e}{e n_e} - \frac{\vec{u}_e \times \vec{B}}{c} + \frac{m_e \nu_0}{n_e e} \sum_s n_s z_s^2 (\vec{u}_s - \vec{u}_e) \tag{1}$$

where T_e and $\vec{u}_e$ are the electron temperature and drift velocity, $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields, $\vec{J}$ is the total current, n_e is the electron number density, ν_0 is the electron-ion collision frequency, $\vec{u}_s$ is the average ion drift velocity, and z_s is the ion charge state. The plasma is quasi-neutral, $n_e \approx \Sigma_s z_s n_s$. The electron current is $\vec{J}_e = -e n_e \vec{u}_e$. In Hewett's model,[7] the last term in Eq. (1) is replaced by $\overleftrightarrow{\eta} \cdot \vec{J}$, where $\overleftrightarrow{\eta}$ is the resistivity.

By evaluating $\vec{E}$ in Eq. (1) at the advanced time and combining with the equation of magnetostatics,

$$\nabla \times \vec{B} = 4\pi \vec{J}/c \quad , \tag{2}$$

and Faraday's law,

$$\nabla \times \vec{E} = -\partial \vec{B}/c\partial t \quad , \tag{3}$$

Hewett obtains implicit field equations. The ion charge and current densities are gathered explicitly from the particles. At very low densities, Hewett sets $\overleftrightarrow{\eta}$ equal to a large value to force $\nabla \times \vec{B} = 0$. He solves the field equations globally by using a non-iterative alternating-direction-implicit algorithm.

In contrast to Hewett,[7] who solves Eq. (1) for $\vec{E}$, Cohen and Brengle[8] solve for $\vec{u}_e$ and hence, $\vec{J}_e$. Then

$$\hat{\theta} \cdot \nabla^2 \vec{A} = -\frac{4\pi}{c} J_\theta (A_\theta, \phi) \tag{4}$$

globally, and

$$\oint \frac{d\ell}{rB} \frac{\partial}{\partial r} [4\pi r J_r (A_\theta, \phi) - r \frac{\partial^2}{\partial t \partial r} \phi] = 0 \tag{5}$$

on closed magnetic field lines, where $\vec{E} =$ [illegible]$/c\partial t - \hat{r}\partial\phi/\partial r$ and $\vec{B} = \nabla \times A_\theta \hat{\theta}$. Line tying o[illegible] field justifies $\partial\phi/\partial r = 0$. Canonical angular momentum relates the ion current in Eq. (4) to the vector potential A_θ, $\mathcal{P}_{\theta i} \equiv m_i r v_\theta + z_i e r A_\theta$. Equations (4) and (5) are solved iteratively ($\le$ 5 iterations) after linearizing J_θ with respect to A_θ. Temporally averaging J_{ri} over past data reduces statistical noise.

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Both Hewett's[7] and Cohen and Brengle's[8] algorithms avoid potential numerical difficulties arising from the infinite phase velocity of Alfven waves as the mass density approaches zero, $\omega/k = v_A \equiv (B^2/4\pi n m_i)^{1/2} \to \infty$. In these implicit hybrid codes, the stability condition $\Delta x/\Delta t > v_A$ is relaxed. Time-step constraints are set instead by accuracy considerations and stability of the ion orbits.[7,8]

Implicit Moment Equations. Mason[1] and Denavit[2] independently synthesized simulation schemes whose implicitness is derived from the introduction of fluid moment equations. This improves the hybrid models in that all species are now kinetic and implicitly coupled to the fields. The implicit moment method has robust stability properties and is broadly applicable.

In a one-dimensional electrostatic model, the fluid equations in difference form are

$$\tilde{n}_s^{n+1} = n_s^n - \Delta t D_x \tilde{J}_s^{n+1/2}/q_s \; ; \qquad (6)$$

$$\tilde{J}_s^{n+1/2} = J_s^{n-1/2} + q_s \Delta t(-D_x P_s^{\dagger n} + q_s n_s^n E^*)/m_s \; , \qquad (7)$$

where $P_s^\dagger = \Delta x^{-1}\sum_j m_s v_j^2$ is the kinetic stress summed over the particles, D_x is the difference form of $\partial/\partial x$, $\tilde{n}_s$ and $\tilde{J}_s$ are implicit predictions of the fluid number and current densities, n_s and J_s are the explicit densities accumulated from the particles, and

$$E^* = \theta E^{n+1} + \frac{(1-\theta)}{4}(E^{n+1}+2E^n+E^{n-1}) \; ; \; 0 \le \theta \le 1 \; . \qquad (8)$$

The electric field is calculated from Gauss' law

$$D_x E^{n+1} = 4\pi \sum q_s n_s^{n+1} \quad , \qquad (9)$$

rendered implicit by use of Eqs. (6) and (7). Particles are then advanced individually with the implicitly predicted electric field, and the necessary particle data are gathered.

An iteration can be performed to better time-center $P_s^\dagger$, whose convergence requires[2]

$$k v \Delta t < 1 \quad , \qquad (10)$$

where v is a characteristic particle velocity and k is the largest wave number retained. This is also the condition for accurate particle trajectories and plasma dielectric response.[5,9] The implicit field solution relaxes the stability constraint set by plasma waves, allowing $\Delta t > \omega_p^{-1}$, the inverse plasma frequency. With $\omega_p \Delta t > 1$, Eq. (10) restricts wavelengths to be long compared to the Debye length,

$$k\lambda_D \equiv k(T/4\pi n e^2)^{1/2} = k v_t \Delta t/\omega_p \Delta t << 1 \quad , \qquad (11)$$

where $v_t \equiv (T/m)^{1/2}$. An implicit prediction of the kinetic stress relaxes the $kv\Delta t$ stability constraint,[1,6] but does not remove it as an accuracy constraint.[5,9]

For $\omega_p \Delta t << 1$ and $\Delta x > \lambda_D$, there can be a grid-aliasing instability,[14] which results in heating until $\lambda_D \sim \Delta x$. However, implicitness, dissipation,[5] and use of $\omega_p \Delta t > 1$, or a change of the force law,[14] control the grid instability.[2,6] Thus, for $\Delta x >> \lambda_D$, the timestep in the implicit moment algorithm is bounded from above by Eq. (10) and from below by the finite-grid instability. These limits are not a serious hindrance.[1,2,6]

Mason[1] and Denavit[2] have successfully applied this scheme to a number of problems. Of importance are simulations of electron transport in inertial-confinement fusion.[15] Brackbill and Forslund[6] have extended the implicit moment method to impressive two-dimensional electromagnetic simulations of the Weibel and lower-hybrid-drift instabilities, shocks, and collisionless electron transport in laser fusion.[6] The implicit moment method has been applied by Barnes and Kamimura[16] to two-dimensional, electrostatic simulations of low-frequency phenomena in magnetized plasma using both guiding-center and Newton-Lorentz particle equations. J. A. Byers has applied the moment method to linearized electrostatic simulations of unstable Bernstein waves (unpublished).

III. Direct Implicit Particle Methods

In the direct implicit particle method,[3,9] an implicit solution of the field equations is achieved by relating a linear increment to the charge and current density directly to the change in the particle motion induced by the fields or their increments at the advanced time. This differs markedly from the implicit moment method, but the two methods possess similar stability and accuracy properties.[5,9]

In a simple one-dimensional electrostatic model,[3] the direct implicit method has the following form. The particle position x^{n+1} at time t^{n+1} is

$$x^{n+1} = \beta \Delta t^2 a^{n+1} + \tilde{x}^{n+1} \quad , \qquad (12)$$

where $0 < \beta < 1$ and $\tilde{x}^{n+1}$ is the position with a^{n+1} suppressed in the equation of motion. Thus, $x^{n+1} = \tilde{x}^{n+1} + \delta x$, where $\delta x = \beta \Delta t^2 a^{n+1}$; and the charge density is $\rho^{n+1} = \tilde{\rho}^{n+1}(\tilde{x}^{n+1}) + \delta\rho$, where

$$\delta\rho = -\nabla\cdot[\tilde{\rho}^{n+1}(x)\, \delta\tilde{x}(x)] \qquad (13)$$

is the linearized increment to the charge density. Poisson's equation gives

$$-\nabla\cdot(1+\chi)\nabla\phi^{n+1} = \tilde{\rho}^{n+1} \quad , \qquad (14)$$

where the effective susceptibility is

$$\chi(x) = 4\pi\beta(q\tilde{\rho}^{n+1}/m)\Delta t^2 = \beta\, \omega_p^2(x)\Delta t^2 \quad . \qquad (15)$$

The charge density is related to the particle positions by

$$\rho_j^{n+1} = (q/\Delta x)\sum_k S(x_k^{n+1} - x_j) \quad , \qquad (16)$$

where j is the grid index, k is the particle index, q is the charge, and S is the "shape function" for particle-mesh interpolation. Expanding S gives

$$S(x_k^{n+1}-x_j) = S(\tilde{x}_k^{n+1} - x_j) + (x_k^{n+1}-\tilde{x}_k^{n+1})\frac{\partial S(\tilde{x}_k^{n+1}-x_j)}{\partial \tilde{x}_k^{n+1}} \; , \qquad (17)$$

and from Eq. (12)

$$x_k^{n+1} - \tilde{x}_k^{n+1} \simeq (q/m)\Delta t^2 \sum_i S(\tilde{x}_k^{n+1} - x_i)E_i^{n+1} \qquad (18)$$

with relative error of order $\omega_{tr}^2 \Delta t^2 = qE\Delta t^2/mL_E < 1$, where ω_{tr} is the particle trapping frequency and L_E is the length scale over which E varies.

With the use of Eqs. (14), (17), and (18), Poisson's equation becomes

$$-(\phi_{j-1}^{n+1} - 2\phi_j^{n+1} + \phi_{j+1}^{n+1})/\Delta x^2 = 4\pi\tilde{\rho}_j^{n+1} + \sum_i W_{ij}E_i^{n+1} \quad , \qquad (19)$$

where $\tilde{\rho}_j^{n+1}$ is the conventional charge density given by Eq. (17) with $x_k^{n+1} \approx \tilde{x}_k^{n+1}$ and

$$W_{ij} = \frac{4\pi q^2 \Delta t^2}{m\Delta x}\sum_k S(\tilde{x}_k^{n+1} - x_i)\frac{\partial S(\tilde{x}_k^{n+1} - x_j)}{\partial \tilde{x}_k^{n+1}} \quad . \qquad (20)$$

For linear splines, $W_{ij} = 0$ whenever $|i-j| > 1$ and $\partial S/\partial \tilde{x}_k^{n+1} = \pm 1$ or 0. No additional particle data beyond that needed for $\tilde{\rho}_j^{n+1}$ are needed for W_{ij}, and the field equation is a linear penta-diagonal system solved by direct Gaussian inversion.[3]

The direct method has been tested in simulations of wave propagation, two-stream instability, and free expansion of a plasma slab; and the implicit difference scheme has been varied.[5,17] If the plasma is nearly uniform so that $\chi(x)$ approximately equals its spatial average, Fourier transform methods can be used.[18]

Langdon, et al.[9] have formulated the direct implicit method with a magnetic field and in two dimensions. The spatial differencing of Eq. (14) can be simplified to reduce the bandedness of the matrix equation for the field. Langdon, et al.[9] address the subtle problem of self-consistent spatial filtering and also prove that the implicit field-particle matrix equation is positive and in some cases symmetric, useful properties for iterative solutions. Reference (9) also outlines a simple iteration scheme to obtain a more exact solution of Poisson's equation.

The direct method relaxes the usual stability constraint on $\omega_p \Delta t$. Where $kv_t \Delta t < 1$ is a stability constraint in the implicit moment method, $\omega_{tr} \Delta t < 1$ is required in the direct method. However, $kv_t \Delta t < 1$ remains as an accuracy constraint; and the grid-aliasing instability must be controlled. Finally, the direct method avoids the possible difficulty in the implicit moment method that the fluid number and current densities are inconsistent with those accumulated from the particles.

IV. Orbit-Averaged Implicit Codes

Orbit averaging[10,11] and subcycling[12] take a multiple time-scale approach to particle simulation. Independent time scales are selected for advancing particles and fields according to natural separations that exist. The subcycling method succeeds in making the ions a negligible factor in the cost of simulating ions and electrons.[12] However, the algorithm described in Ref. (12) is explicit and therefore does not allow the use of a large $\omega_{pe} \Delta t$.

Orbit averaging[10,11] differs from subcycling and is more complicated. In its original magneto-inductive form,[10] a particle species gyrating in a magnetic field is explicitly advanced with a small timestep, $\omega_c \Delta t < 1$ where $\omega_c \equiv qB/mc$. Currents are accumulated on a spatial grid after each small time-step and are temporally averaged over ΔT, $\omega_c \Delta T >> 1$, for use in Ampere's law to determine the vector potential and magnetic field. An inductive electric field is calculated from Faraday's law, and electro-statics are ignored. The fields are advanced with the large timestep. A corrector iteration through the particle and field equations is performed to improve the time centering. Biasing of the field equations to the field amplitudes at the advanced time level introduces dissipation.

Analysis and simulations show that the orbit-averaged magneto-inductive scheme, although explicit, is numerically stable with use of large ΔT: $\Delta T >> \Delta t$, $\omega_c \Delta T >> 1$, and $kv_A \Delta T >> 1$.[10] However, this scheme is unstable for $kv_A \Delta T \leq \mathcal{O}(1)$. The real triumph of orbit averaging is how it significantly reduces the number of particles and total operations: the averaged contributions from a single particle can substitute for those from many particles in a conventional code. This increased efficiency has allowed realistic two-dimensional simulations of mirror experiments at Lawrence Livermore National Laboratory.[10]

In contrast to the magneto-inductive algorithm, stability of an orbit-averaged electrostatic algorithm for $\omega_p \Delta T > 1$ requires implicit solution of Poisson's equation.[11] The combination of orbit averaging with the direct implicit and implicit moment methods can produce algorithms that are stable for $\omega_p \Delta T > 1$.[11] Orbit averaging in this application achieves a reduction of particles and allows the particles to be advanced serially over many timesteps before incurring input/output penalties, an advantage for large simulations using disk storage. Even greater gains in efficiency can be achieved with a better separation of particle and field timesteps, by using an implicit prediction of the kinet[illegible] stress[6] or when wave propagation is perpendicul[illegible] to $\vec{B}$.[11]

V. General Consideration[illegible] and Futur[illegible] [illegible]irections

In developing new imp[illegible]t difference schemes for particle simulation, des[illegible] criteria have evolved:

- Accurate reproduction of low-frequency phenomena $\omega_0 < \Delta t^{-1}$, e.g., $\mathrm{Im}(\omega/\omega_0)$ should be minimal.
- Substantial damping of modes with $\omega_0 > \Delta t^{-1}$.
- Minimal collection and storage of particle data.
- Minimal numerical cooling and heating.[5]
- Galilean invariance so as not to destabilize fast or slow space-charge waves.[5]
- Robust stability and accuracy properties with respect to approximate solution for the fields.

Analyses of wave dispersion properties in Refs. (2), (5), and (6) have led to a number of important conclusions. With proper choice of coefficients in the differencing schemes,[5] damping of high-frequency oscillations $\omega_0 \Delta t \geq 1$ can be enhanced, while the damping of low-frequency waves can be removed to high order in $\omega_0 \Delta t < 1$. The wave dissipation properties and unphysical secular particle acceleration are directly related.[5]

Both implicit moment and direct implicit algorithms have proven successful in performing simulations with large timestep. Magnetic fields have been incorporated,[5,6,9] and iterative refinement of the solution of the implicit field-particle equations has been studied.[1,2,9] The two methods share residual constraints on the timestep that generally coincide with those required to resolve physical processes, e.g., $k\lambda_D < 1$, $kv_t \Delta t < 1$.[2,5,6,9]

Research on implicit particle codes continues. Areas of interest are numerous. It would be desirable to relax residual constraints. The problem of self-consistent spatial smoothing[9] has not been resolved. The potential for (and limitations of) simplified spatial differencing should be examined. More simulation experience is needed, especially with direct implicit and orbit-averaged algorithms. Two-dimensional and electromagnetic (and possibly relativistic) direct implicit simulations should be undertaken. More needs to be done on how to best realize additional computational savings by combining orbit-averaging or subcycling with implicit methods. Research continues, motivated by the impressive successes of these new techniques in dramatically extending the applicability of particle simulations and greatly improving their realism.[6,10,15]

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References

1. R.J. Mason, J. Comp. Phys. 41, 233 (1981).
2. J. Denavit, J. Comp. Phys. 42, 337 (1981).
3. A. Friedman, A.B. Langdon, and B.I. Cohen, Comments Plasma Phys. Contr. Fusion 6, 225 (1981).
4. A.B. Langdon, J. Comp. Phys. 30, 202 (1979).
5. B.I. Cohen, A.B. Langdon, and A. Friedman, J. Comp. Phys. (in press).
6. J.U. Brackbill and D.W. Forslund, Bull. Am. Phys. Soc. 26, 1010 (1981); J. Comp. Phys. and Phys. Rev. Lett. (in press).
7. D.W. Hewett, J. Comp. Phys. 38, 378 (1980).
8. B.I. Cohen and T.A. Brengle, in Proceedings Controlled Fusion Theory Conference (University of Texas, Austin, 1981), paper 2B14.
9. A.B. Langdon, B.I. Cohen, and A. Friedman, submitted to J. Comp. Phys.
10. B.I. Cohen, T.A. Brengle, D.B. Conley, and R.P. Freis, J. Comp. Phys. 38, 45 (1980); B.I. Cohen and R.P. Freis, J. Comp. Phys. in press.
11. B.I. Cohen, R.P. Freis, and V. Thomas, J. Comp. Phys. (in press).
12. J.C. Adam, A. Gourdin Serveniere, and A.B. Langdon, submitted to J. Comp. Phys.
13. W.W. Lee, submitted to J. Comp. Phys.
14. A.B. Langdon, J. Comp. Phys. 6, 247 (1970).
15. R.J. Mason, Phys. Rev. Lett. 47, 652 (1981).
16. D.C. Barnes and T. Kamimura, Bull. Am. Phys. Soc. 26, 986 (1981), paper 6R8.
17. A. Friedman, A.B. Langdon, and B.I. Cohen, Bull. Am. Phys. Soc. 26, 985 (1981), paper 6R2.
18. T. Tajima and J.N. Leboeuf, Bull. Am. Phys. Soc. 26, 986 (1981), paper 6R9.