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Note

Semi-Implicit Particle Simulation of Kinetic Plasma Phenomena

1. INTRODUCTION

This paper presents recent progress in improving the efficiency of particle simulations of kinetic plasma phenomena when there are disparate time scales. Kinetic phenomena in plasmas exhibit ranges of time and space scales that span many orders of magnitude [1]. If the physical phenomenon of interest possesses characteristic time and space scales that represent a much slower variation than that of the most rapid variations admitted by the fundamental equations describing the system, then the system of equations is stiff. A large disparity in time and space scales places great stress on the numerical methods used to simulate such a system. This is a classic problem in computational physics and has received much attention. This paper presents a new advance in rendering particle simulation of plasmas more efficient by means of a semi-implicit integration technique. A general class of physics models is amenable to semi-implicit integration, and implementation of the scheme is simple and straightforward. The technique is illustrated here with model algorithms and numerical dispersion analyses. We demonstrate that the desirable accuracy and stability characteristics of a class of direct implicit particle schemes introduced earlier [2, 3] can be recovered with the semi-implicit algorithm. Furthermore, the semi-implicit method is easily adapted to electron subcycling [4] and orbit-averaging [5] and circumvents some difficulties identified in combining implicitness with orbit-averaging [6]. In electron subcycling, the electron equations of motion and the field equation(s) are advanced with the same timestep; and the ion equations of motion are advanced less often with a bigger timestep. In an orbit-averaged algorithm, the equations of motion of one or more plasma species are advanced with a small timestep; the contributions to the plasma charge and current densities are time-averaged; and the field equations are solved with a larger timestep.

The new invention reported here is a natural outgrowth of the developments that have been made in implicit and other multiple-timescale techniques used in plasma simulation [7]. Of particular importance in motivating the present work was the successful introductrion of the semi-implicit magnetohydrodynamic simulation method by Harned and Kerner [8]. In the semi-implicit method, additional terms

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are introduced into the finite-difference equations, usually as the difference of two expressions that differ only in the time level of the dependent field or fluid variable. The form of the additional terms is dictated by the structure of the difference equations and the characteristics of the normal modes. To illustrate this, consider the following elementary finite-difference equation describing a harmonic oscillator:

$$x_{n+1} - 2x_n + x_{n-1} = -\omega_0^2 \Delta t^2 x_n. \tag{1}$$

This difference equation has the driving force on the right side expressed as an explicit function of the displacement. With the right side replaced with the centered implicit expression $-\omega_0^2 \Delta t^2 (x_{n+1} + 2x_n + x_{n-1})/4$, unconditional stability for $\omega_0^2 \Delta t^2 \gg 1$ is achieved while maintaining second-order accuracy in time for $\omega_0^2 \Delta t^2 \ll 1$. The semi-implicit form of Eq. (1) can be obtained by adding the following expression to the right side of (1):

$$\omega_0^2 \Delta t^2 [x_n - (x_{n+1} + 2x_n + x_{n-1})/4] \tag{2a}$$

or, equivalently,

$$\omega_0^2 \Delta t^2 [(x_n - x_{n+1}) - (x_{n-1} - x_n)]/4. \tag{2b}$$

This example displays the essence of a semi-implicit integration scheme. To implement it in a particle simulation, we shall identify the correct expressions to subtract and add to the field equations in the simulation algorithm to render it semi-implicit. The choice of expressions is guided by analyzing the numerical dispersion of the algorithm. Finally, past experience and analysis of implicit particle algorithms dictate the appropriate choreography of particle-pushing and field-solving steps to achieve the desired stability and accuracy characteristics [2, 3]. This will be made explicit in the following discussion of algorithms and stability analyses.

The earlier work of Cohen, Freis, and Thomas [6] addressed the closely related issue of merging implicit particle methods with orbit averaging. That work suggested that both direct implicit and implicit moments methods could be combined with orbit averaging to yield algorithms that were stable at large timestep. However, only the orbit-averaged, implicit moment algorithm was demonstrated in [6]; and Cohen [1] suggested that the resulting matrix equation for the field in an orbit-averaged, direct implicit algorithm might lose its sparseness. Furthermore, an orbit-averaged, direct implicit algorithm has never been demonstrated in a working code. The new work here introduces semi-implicit methods to particle simulation and shows how subcycling and orbit averaging are easily incorporated without changing the sparseness pattern of the matrix field equations.

The rest of the paper is organized as follows. Section 2 presents a semi-implicit electrostatic algorithm for an unmagnetized plasma and the associated numerical dispersion analysis. The dispersion relation of a class of direct-implicit algorithms analyzed in [3] is recovered. In Section 3 a semi-implicit, orbit-averaged, electrostatic algorithm is introduced; and its dispersion relation is derived. A semi-implicit, orbit-averaged, electrostatic gyrokinetic [9] algorithm is presented and analyzed in Section 4. Conclusions are given in Section 5.

2. Semi-Implicit Electrostatic Particle Algorithm

Consider the following variation of a simple leapfrog electrostatic particle algorithm. The electron velocities $\mathbf{v}$ and positions $\mathbf{x}$ are advanced according to

$$\mathbf{v}_{n+1/2} = \mathbf{v}_{n-1/2} + \Delta t\, \mathbf{a}_n \tag{3a}$$

$$\tilde{\mathbf{x}}_{n+1} = \mathbf{x}_n + \Delta t\, \mathbf{v}_{n+1/2}, \tag{3b}$$

where $\mathbf{a}_n$ is the particle acceleration as calculated by interpolating the electromagnetic forces from the grid to the particle, and the subscripts denote the time levels. If we ignore the modifications due to introducing a grid, then the acceleration in an unmagnetized plasma is just $\mathbf{a}_n = -(q/m)\nabla\phi_n$. A time-centered $\mathbf{v}\times\mathbf{B}$ Lorentz force can be straightforwardly included to accommodate an applied magnetic field. From the temporary values $\{\tilde{\mathbf{x}}_{n+1}\}$, an electron density $\tilde{n}_{n+1}$ is accumulated on the grid using the same interpolation scheme as for the force on the particle, but in the reverse direction. Poisson's equation is then solved to determine the self-consistent electric potential. If we again disregard modifications to account for finite-differencing on a grid, a general class of semi-implicit Poisson equations can be cast in the form

$$\begin{aligned} -\nabla^2\phi_{n+1} &= 4\pi e(n_0 - \tilde{n}_{n+1}) \\ &\quad + \nabla\cdot\{\omega_{pe}^2\,\Delta t^2\,\nabla[C_0(\phi_n - \phi_{n+1}) + C_1(\phi_{n-1} - \phi_n) + \cdots]\}, \end{aligned} \tag{4}$$

where the constants $\{C_i\}$ are chosen to optimize certain properties of the integration scheme [10, 3]. The term in the Poisson equation containing the time series in ϕ_n constitutes the semi-implicit modification of the field equation. Effects due to interpolation between the particles and the grid, and due to finite differencing have been omitted throughout to simplify the presentation; but these effects could be included quite straightforwardly without fundamentally changing the results given here.

Because of the semi-implicit modification of Poisson's equation, the force term used in the velocity advance is no longer consistent with the effective electron charge density used in (4). To remedy this, a corrector advance of the electron displacements is computed:

$$\mathbf{x}_{n+1} = \tilde{\mathbf{x}}_{n+1} + C_0(\mathbf{a}_{n+1} - \mathbf{a}_n)\,\Delta t^2 + C_1(\mathbf{a}_n - \mathbf{a}_{n-1})\,\Delta t^2 + \cdots. \tag{5}$$

The explicit form of the correction terms on the right side of Eq. (5) is derived by analytically calculating the linear increment to the charge density that they induce and constraining it to match the semi-implicit term in Eq. (4).

To study the temporal stability and accuracy of this algorithm, we derive the linear dispersion relation describing the normal modes of the difference equations using standard techniques [3]. First, Eq. (3b) is used to algebraically eliminate $\tilde{\mathbf{x}}_{n+1}$. Equations (3a), (4), and (5) are linearized next and Fourier analyzed in time

and space; and the amplification factor $\lambda = \phi_{n+1}/\phi_n = \exp(-i\omega\,\Delta t)$ is introduced. The linearly perturbed electron charge density in a cold, non-drifting, uniform plasma can be shown to be $en_0 i\mathbf{k}\cdot\mathbf{x}(\omega)$, where $\mathbf{x}(\omega)$ is the Fourier amplitude of the linear displacement. These steps reduce Eqs. (3a), (4), and (5) to a linear system of equations for the Fourier amplitudes $\mathbf{x}(\omega)$, $\mathbf{v}(\omega)$, and $\phi(\omega)$, whose characteristic equation yields the dispersion relation

$$\frac{1}{\omega_{pe}^2\,\Delta t^2} + \frac{\lambda}{(\lambda-1)^2} + C_0 + \frac{C_1}{\lambda} + \frac{C_2}{\lambda^2} + \cdots = 0, \tag{6}$$

in the absence of grid corrections; ω_{pe} is the plasma frequency. This recovers the dispersion relation derived by Cohen, Langdon, and Friedman in [3] for the class C direct implicit schemes.

The influence of finite differencing and spatial interpolation to a grid on the direct implicit algorithms was analyzed in [11, 12]. It is straightforward to include finite-differencing and grid interpolation effects in a semi-implicit algorithm in such a way as to mimic the same linear dispersion derived in [11, 12]. The methods for this are derived from the techniques used in [11, 12]. Some aspects of the dispersion of the direct implicit algorithm for both a drifting plasma and a cold, non-drifting, magnetized plasma were analyzed in [3]; some warm plasma effects were addressed analytically in [11] and in the direct implicit simulations of a hot, expanding plasma slab in [13]. Based on the analysis and arguments presented here and previous experience, we expect that the semi-implicit algorithm will have dispersion properties that are very similar to the direct implicit method in most respects.

The dispersion relation in Eq. (6) describes plasma oscillations. The analysis in [3] demonstrated how numerical stability could be maintained for a subset of the C schemes with $C_0 + 1/\omega_{pe}^2\,\Delta t^2 > C_1 + \frac{1}{4}$ and $C_{i\geqslant 2} = 0$ (C_1 scheme). The C schemes are second-order accurate in time for $\omega_{pe}^2\,\Delta t^2 \ll 1$, and dissipation is introduced when $C_{i\geqslant 1} > 0$. Figures 1 and 2 in [3] provide more detailed results on the stability and dissipation in the C_1 scheme. There is considerable experience in using the C_1 scheme [13]. The conclusion of this section is that the desirable dispersion properties of the C_1 direct implicit algorithm can be recovered in a semi-implicit algorithm.

3. Semi-Implicit, Orbit-Averaged, Electrostatic Algorithm

Earlier work reported in [6] demonstrated that an orbit-averaged electrostatic algorithm was subject to a timestep constraint to ensure numerical stability. Numerical stability at large timestep could be achieved in an implicit, orbit-averaged algorithm. This was demonstrated in [6] where orbit averaging was combined with the implicit moment method. It was unclear whether orbit averaging could be combined with the direct implicit method so that the matrix equation for

the implicit Poisson's equation remained banded and sparse. Here we present a semi-implicit, orbit-averaged, electrostatic algorithm leading to a field equation that is sparse and banded. This algorithm is attractive for several reasons. The use of a large timestep in the field solution and the ion advance improves the efficiency of simulating slowly evolving collective phenomena. In addition, the orbit averaging of the electrons facilitates using both a small timestep to accurately resolve the electron trajectories and a reduced number of electrons to statistically sample the velocity distribution function.

In an orbit-averaged algorithm, the electrons are advanced from $N\,\Delta T$ to $(N+1)\,\Delta T$ starting at $\{\mathbf{x}_N, \mathbf{v}_N\}$ with small timesteps $\Delta t \ll \Delta T$:

$$\tilde{\mathbf{v}}_{n+1/2} = \tilde{\mathbf{v}}_{n-1/2} + \mathbf{a}^e_N\,\Delta t \tag{7a}$$

$$\tilde{\mathbf{x}}_{n+1} = \tilde{\mathbf{x}}_n + \tilde{\mathbf{v}}_{n+1/2}\,\Delta t, \tag{7b}$$

where n is the index for the small timestep advance, N is the index of the time level for the field solution and ion advance, and $\mathbf{a}^e_N = -(q/m)\nabla\phi_N$ is the acceleration evaluated at the particle position $\tilde{\mathbf{x}}_n$. The $\mathbf{v}\times\mathbf{B}$ Lorentz force could be straightforwardly included. The electron number density n^e_n is accumulated from $\{\tilde{\mathbf{x}}_n\}$ and time-averaged to obtain $\langle n^e\rangle_{N+1/2}$. The current density $\mathbf{J}^e_n$ is accumulated from $\{\tilde{\mathbf{x}}_n, \tilde{\mathbf{v}}_{n-1/2}\}$ and $\{\tilde{\mathbf{x}}_n, \tilde{\mathbf{v}}_{n+1/2}\}$, and averaged in time from $N\,\Delta T$ to $(N+1)\,\Delta T$ to form $\langle \mathbf{J}^e\rangle_{N+1/2}$. Ions can be advanced in conventional leapfrog fashion with the field solve interleaved:

$$\mathbf{V}_{N+1/2} = \mathbf{V}_{N-1/2} + \mathbf{a}^i_N\,\Delta T \tag{8a}$$

$$\mathbf{X}_{N+1} = \mathbf{X}_N + \mathbf{V}_{N+1/2}\,\Delta T. \tag{8b}$$

The ion number density n^i_{N+1} is accumulated from $\{\mathbf{X}_{n+1}\}$.

The semi-implicit Poisson equation is motivated by the results presented in [6],

$$\begin{aligned}-\nabla^2(\phi_{N+1}-\phi_N) = &-4\pi\,\Delta T\nabla\cdot\langle\mathbf{J}^e\rangle_{N+1/2} + 4\pi e(n^i_{N+1}-n^i_N)\\ &+\nabla\cdot\{\bar{\omega}^2_{pe}\,\Delta T^2[C_0(\nabla\phi_{N+1}-\nabla\phi_N)\\ &+C_1(\nabla\phi_N-\nabla\phi_{N-1})+\cdots]\},\end{aligned} \tag{9}$$

where $\bar{\omega}^2_{pe} = 4\pi\langle n^e\rangle_{N+1/2}\,e^2/m_e$. In order for the electron trajectories to be consistent with the charge density appearing in Eq. (9), an electron corrector advance must be undertaken from $N\,\Delta T$ to $(N+1)\,\Delta T$:

$$\mathbf{v}_{n+1/2} = \mathbf{v}_{n-1/2} + \Delta t[\mathbf{a}^e_N + 2C_0(\mathbf{a}^e_{N+1}-\mathbf{a}^e_N)+\cdots], \tag{10a}$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}_{n+1/2}\,\Delta t, \tag{10b}$$

where the accelerations in (10a) are computed at the $\mathbf{x}_n$ particle positions. The electron number and current densities are *not* collected on the corrector pass. The semi-implicit Poisson equation, Eq. (9), leads to a sparse, banded matrix equation with

the same structure as the field solution for the direct implicit method with simplified spatial differencing [2, 11, 12].

The analysis of the linear dispersion relation for this semi-implicit, orbit-averaged, electrostatic algorithm and the demonstration of its numerical stability for $\omega_{pe}\,\Delta T \gg 1$ are similar to the dispersion analysis in Section 2. We again consider linear waves in a uniform, cold, non-drifting plasma. For the electron plasma wave branch, the ions can be assumed to be stationary. The linearized quantities $\tilde{\mathbf{x}}_{n+1}$ and $\tilde{\mathbf{v}}_{n+1/2}$ can be eliminated algebraically:

$$\tilde{\mathbf{x}}_{n+1} = \mathbf{x}_N + \mathbf{v}_N(n+1)\,\Delta t + \mathbf{a}_N \frac{(n+1)n}{2}\,\Delta t^2, \qquad \tilde{\mathbf{v}}_{n+1/2} = \mathbf{v}_N + \mathbf{a}_N(n+1)\,\Delta t. \tag{11}$$

The linearized orbit-averaged current is determined from $\{\tilde{\mathbf{v}}_{n+1/2}\}$:

$$\langle \mathbf{J}^e \rangle_{N+1/2} = -n_0 e\left[\mathbf{v}_N - \left(\frac{e}{2m_e}\right)\Delta T \mathbf{E}_N\right]. \tag{12}$$

The linearized electron corrector equations can be solved in similar fashion to Eq. (11) to obtain

$$\begin{aligned} \mathbf{x}_{n+1} &= \mathbf{x}_N + \mathbf{v}_N(n+1)\,\Delta t + \frac{(n+1)n}{2}\,\Delta t^2[\mathbf{a}_N + 2C_0(\mathbf{a}_{mN+1} - \mathbf{a}_{mN}) + \cdots], \\ \mathbf{v}_{n+1/2} &= \mathbf{v}_N + (n+1)\,\Delta t[\mathbf{a}_N + 2C_0(\mathbf{a}_{N+1} - \mathbf{a}_N) + \cdots]. \end{aligned} \tag{13}$$

If we assume $\Delta T \gg \Delta t$, evaluate $(\mathbf{x}_n, \mathbf{v}_{n+1/2})$ at $(N+1)\,\Delta T$, Fourier transform in time, and consider $C_0 \neq 0$ and $C_{i\geq 1} = 0$, we obtain

$$(\lambda - 1)\mathbf{k}\cdot\mathbf{v}(\omega) = -\frac{e}{m_e}\,\Delta T[2C_0\lambda + (1 - 2C_0)]\mathbf{k}\cdot\mathbf{E}(\omega), \tag{14}$$

where $\lambda = \exp(-i\omega\,\Delta T)$. We Fourier analyze the linearized orbit-averaged current in Eq. (12) and substitute it into Poisson's equation, Eq. (9), to obtain

$$\begin{aligned} (\lambda - 1)\mathbf{k}\cdot\mathbf{E}(\omega) = 4\pi e n_0\,\Delta T \mathbf{k}\cdot\left[\mathbf{v}(\omega) - \left(\frac{e}{m_e}\right)\Delta T\frac{\mathbf{E}(\omega)}{2}\right] \\ + C_0\omega_{pe}^2\,\Delta T^2(1-\lambda)\mathbf{k}\cdot\mathbf{E}(\omega). \end{aligned} \tag{15}$$

A dispersion relation is then obtained by algebraically eliminating $\mathbf{k}\cdot\mathbf{v}(\omega)$ and $\mathbf{k}\cdot\mathbf{E}(\omega)$ from Eqs. (14) and (15):

$$(1 + C_0\omega_{pe}^2\,\Delta T^2)(\lambda - 1)^2 + \omega_{pe}^2\,\Delta T^2[(2C_0 + 1/2)(\lambda - 1) + 1] = 0. \tag{16}$$

In the limit $\omega_{pe}^2\,\Delta T^2 \gg 1$, the two solutions of Eq. (16) are $\lambda = 1 - 1/(2C_0)$, and $-1 + O(1/\omega_{pe}^2\,\Delta T^2)$, which are stable ($|\lambda| < 1$) for $C_0 > \frac{1}{4}$. For $\omega_{pe}^2\,\Delta T^2 \ll 1$ and

$C_0 > \frac{1}{4}$, the two solutions of Eq. (16) are damped electron plasma oscillations, $\mathrm{Re}(\omega) \approx \pm\omega_{pe}$, with relative damping rate proportional to $(C_0 - \frac{1}{4})\,\omega_{pe}\,\Delta T$ and frequency shift proportional to $\omega_{pe}^2\,\Delta T^2$.

4. Orbit-Averaged, Semi-Implicit Gyrokinetic Algorithm

Gyrokinetic particle simulation [9] has proven itself to be an important tool in studying drift-wave instabilities and the concomitant turbulent transport. Gyrokinetics is a systematic scheme for reducing the Vlasov–Maxwell or Vlasov–Poisson equations to a low-frequency limit that is valid for frequencies much lower than the cyclotron frequency and for waves with $k_{||} \ll k_\perp$ ($k_{||}$ is the wavenumber component parallel to the applied magnetic field and $k_\perp$ is the perpendicular component), but with $k_\perp \bar{\rho}_i \leqslant O(1)$, where $\bar{\rho}_i$ is the ion Larmor radius of a thermal ion. When conventional particle simulation techniques are used to simulate low-frequency waves with $k_\perp \bar{\rho}_i = O(1)$, the ion cyclotron time scale must be resolved, which results in the use of timesteps that can be several orders of magnitude smaller than the periods of the drift waves that are thought to be responsible for anomalous transport in magnetic fusion devices. Gyrokinetic simulation does not have to resolve the ion cyclotron time scale, and a much larger timestep can be used than in a conventional simulation. However, a significant separation in electron and ion time scales persists in electrostatic gyrokinetic particle simulation with kinetic electrons; and this circumstance provides an opportunity for the application of orbit averaging and semi-implicit integration to further improve the efficiency of drift-wave simulation.

In a conventional gyrokinetic algorithm with kinetic electrons and ions, the hierarchy of time scales is as follows. The highest frequency normal mode has a frequency $\omega_h = (m_i/m_e)^{1/2}\,(k_{||}/k_\perp)\Omega_i$ in the limit $\omega_{pi}^2/\Omega_i^2 \gg 1$, where $\Omega_i = eB_0/m_i c$ is the ion cyclotron frequency. The timestep Δt must satisfy $\omega_h\,\Delta t < O(1)$ to ensure numerical stability. In order to accurately track the electron trajectories, one must also guarantee $k_{||} v_e\,\Delta t < 1$, where $k_{||} v_e = (T_e/T_i)^{1/2}\,k_\perp \bar{\rho}_i \omega_h$ is the parallel transit frequency (which has been related algebraically to ω_h), v_e is the electron thermal speed, and $\bar{\rho}_i$ is the ion Larmor radius for a thermal ion. For $T_e/T_i = O(1)$ and $k_\perp \bar{\rho}_i = O(1)$, $k_{||} v_e$ and ω_h are comparable. The ion diamagnetic drift frequency $\omega_*^i = k_y \bar{\rho}_i (\bar{\rho}_i/L_n)\Omega_i$ and the ion parallel transit frequency $k_{||} v_i = (m_e/m_i)^{1/2}\,(T_i/T_e)^{1/2}\,k_{||} v_e$ represent much slower temporal variations. These conditions invite the use of a method like implicit orbit averaging that will take advantage of the disparity in time scales between the relatively fast electron motion parallel to the magnetic field lines and the slower ion motion and drift waves. A smaller timestep can be assigned to the electron advance, and a bigger timestep can be used for the ion advance and the field solution. Inspired by the earlier success with orbit averaging [5], we hope that orbit averaging will reduce the statistical requirements on the electrons in the gyrokinetic model. Finally, the implicitness will ensure numerical stability.

A semi-implicit, orbit-averaged, electrostatic gyrokinetic algorithm can be constructed following the example presented in Section 3. The algorithm consists of equations that are consistently ordered through the lowest significant order in the gyrokinetic expansion parameter ε, where $k_{||}/k_{\perp}$, $k_{\perp}\bar{\rho}_i e\phi/T_e$, ω/Ω_i, $\bar{\rho}_i/L_n = O(\varepsilon)$ and $k_{\perp}\bar{\rho}_i \leqslant O(1)$. These equations lead to a conserved, energy-like quantity that is equal to the energy invariant derived by Dubin and co-workers [14] through second order in ε. The electrons are advanced in a predictor step from $N\Delta T$ to $(N+1)\Delta T$ using the equations

$$\tilde{v}_{||n+1/2} = \tilde{v}_{||n-1/2} - \left(\frac{e}{m_e}\right)\Delta t\, \mathbf{E}_N \cdot \hat{\mathbf{b}} \tag{17a}$$

$$\tilde{\mathbf{v}}_{\perp n} = c\frac{\mathbf{E}_N \times \hat{\mathbf{b}}}{B_0} \tag{17b}$$

$$\tilde{\mathbf{x}}_{n+1} = \tilde{\mathbf{x}}_n + \tilde{\mathbf{v}}_{n+1/2}\,\Delta t, \tag{17c}$$

where n is the index for the small timestep advance, $\hat{\mathbf{b}} = \mathbf{B}_0/B_0$, N is the index for the field solution and ion advance timestep, $\mathbf{E}_N = -\nabla\phi_N$, the electric field is evaluated at the electron guiding center position $\tilde{\mathbf{x}}_n$ (the electron Larmor radius is negligible), and the starting point is $\{\mathbf{x}_N, \mathbf{v}_N\}$. The electron number and current densities, n_n^e and $\mathbf{J}_n^e$, are calculated at each timestep Δt from $\{\tilde{\mathbf{x}}_n, \tilde{\mathbf{v}}_{n-1/2}\}$ and $\{\tilde{\mathbf{x}}_n, \tilde{\mathbf{v}}_{n+1/2}\}$, and then time-averaged to form $\langle n^e\rangle_{N+1/2}$ and $\langle \mathbf{J}^e\rangle_{N+1/2}$.

The ion gyrocenters are next advanced in a predictor step using the equations

$$\tilde{V}_{||N+1} = \tilde{V}_{||N-1} + 2\Delta T\left(\frac{e}{m_i}\right)\langle \mathbf{E}_N\rangle_{\theta} \cdot \hat{\mathbf{b}} \tag{18a}$$

$$\tilde{\mathbf{V}}_{\perp N} = c\frac{\langle \mathbf{E}_N\rangle_{\theta} \times \hat{\mathbf{b}}}{B_0} \tag{18b}$$

$$\tilde{\mathbf{X}}_{N+1} = \mathbf{X}_{N-1} + 2\Delta T(V_{||N}\hat{\mathbf{b}} + \mathbf{V}_{\perp N}), \tag{18c}$$

where $\langle\ \rangle_{\theta}$ denotes the gyro-averaged quantity. The gyro-averaged ion number density $\tilde{\bar{n}}_{N+1}^i$ is collected from the ion positions displaced by their Larmor radius from $\{\tilde{\mathbf{X}}_{N+1}\}$. A predictor value of the electric potential $\tilde{\phi}_{N+1}$ is determined by the solution of a semi-implicit, gyrokinetic Poisson equation

$$-\left(\nabla^2 + \frac{\omega_{pi}^2}{\Omega_i^2}\, g\, \nabla_{\perp}^2\right)(\tilde{\phi}_{N+1} - \tilde{\phi}_N) = 4\pi e(\tilde{\bar{n}}_{N+1}^i - \bar{n}_N^i) - 4\pi\,\Delta T\nabla \cdot \langle \mathbf{J}^e\rangle_{N+1/2} + C_0\nabla_{||}[\bar{\omega}_{pe}^2\,\Delta T^2\nabla_{||}(\tilde{\phi}_{N+1} - \tilde{\phi}_N)], \tag{19}$$

where $\bar{\omega}_{pe}^2 \equiv 4\pi(e^2/m_e)\langle n^e\rangle_{N+1/2}$, $\bar{\omega}_{pi}^2 = 4\pi n_0 e^2/m_i$, $g = b^{-1}[1 - I_0\exp(-b)]$ in

k-space, and $b \equiv k_\perp^2 \bar{\rho}_i^2$. The ion gyro-centers are then advanced in a corrector step using the equations

$$V_{\|N+1} = V_{\|N} + \Delta T \left(\frac{e}{2m_i}\right) \langle \mathbf{E}^N + \tilde{\mathbf{E}}^{N+1} \rangle_\theta \cdot \hat{\mathbf{b}} \tag{20a}$$

$$\mathbf{V}_{\perp N+1/2} = c \langle \mathbf{E}^N + \tilde{\mathbf{E}}^{N+1} \rangle_\theta \times \frac{\hat{\mathbf{b}}}{2B_0} \tag{20b}$$

$$\mathbf{X}_{N+1} = \mathbf{X}_N + \Delta T \left[\mathbf{V}_{\perp N+1/2} + (V_{\|N+1} + V_{\|N}) \frac{\hat{\mathbf{b}}}{2} \right]. \tag{20c}$$

The corrected gyro-averaged ion density $\bar{n}^i_{N+1}$ is formed from $\{\mathbf{X}_{N+1}\}$ and used in the place of $\tilde{n}^i_{N+1}$ in Eq. (19) to determine ϕ_{N+1}.

The computational step from $N\Delta T$ to $(N+1)\Delta T$ is completed by returning to the electron integration. A corrector pass is calculated starting again at $\{\mathbf{x}_N, \mathbf{v}_N\}$ to guarantee consistency with the time derivative of the total electron charge density on the right side of Eq. (19). The electron corrector advance uses the equations

$$v_{\|n+1/2} = v_{\|n-1/2} - \left(\frac{e}{m_e}\right) \Delta t [\mathbf{E}_N + 2C_0(\mathbf{E}_{N+1} - \mathbf{E}_N)] \cdot \hat{\mathbf{b}} \tag{21a}$$

$$\mathbf{v}_{\perp n+1/2} = c[\mathbf{E}_N + 2C_0(\mathbf{E}_{N+1} - \mathbf{E}_N)] \times \frac{\hat{\mathbf{b}}}{B_0} \tag{21b}$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}_{n+1/2} \Delta t, \tag{21c}$$

where the electric fields are evaluated at $\mathbf{x}_n$. No electron moments need to be computed on the corrector pass through the electrons.

The linear temporal stability analysis for this algorithm is quite analogous to the calculation in Section 3. To simplify the derivation, we consider again the limit of linear waves in a uniform, cold, non-drifting plasma and omit all spatial differencing effects. In this limit, the $\mathbf{E} \times \mathbf{B}$ drift velocities do not lead to any charge separation; and the parallel electron response dominates the ion response. The ion polarization term in Poisson's equation dominates the left side of Eq. (19), and the reduced Poisson's equation becomes

$$-\frac{\omega_{pi}^2}{\Omega_i^2} \nabla_\perp^2 (\phi_{N+1} - \phi_N) \approx -4\pi \Delta T \nabla \cdot \langle \mathbf{J}^e \rangle_{N+1/2} + C_0 \omega_{pe}^2 \Delta T^2 \nabla_\|^2 (\phi_{N+1} - \phi_N). \tag{22}$$

The reduced system of equations, Eqs. (17), (21), and (22), is then identical to the analogous reduction of Eqs. (7)–(10) in Section 3 for the electron plasma-wave

branch with the replacement of $\omega_{pe}^2 \Delta T^2$ with $(k_{||}^2/k_{\perp}^2)(\omega_{pe}^2/\omega_{pi}^2)\,\Omega_i^2 \Delta T^2 = \omega_h^2 \Delta T^2$. Thus, the resulting dispersion relation for the ω_h oscillation is

$$(1 + C_0 \omega_h^2 \Delta T^2)(\lambda - 1)^2 + \omega_h^2 \Delta T^2 [(2C_0 + \tfrac{1}{2})(\lambda - 1) + 1] = 0. \tag{23}$$

For $C_0 > \frac{1}{4}$, there are stable solutions $\lambda = 1 - 1/(2C_0)$ and $-1 + O(1/\omega_h^2 \Delta T^2)$ for $\omega_h^2 \Delta T^2 \gg 1$ and damped oscillations with $\mathrm{Re}(\omega) \approx \pm \omega_h$ for $\omega_h^2 \Delta T^2 \ll 1$.

5. Conclusion

In this paper we have presented the formulation of a new class of semi-implicit algorithms for particle simulation of plasmas. The structure of semi-implicit particle algorithms is relatively simple and is guided by the results of linear numerical dispersion theory for the temporal finite-difference equations. We have shown explicitly that the linear dispersion relation of the direct implicit particle method can be recovered from that of the semi-implicit particle method. Moreover, we have merged semi-implicit integration and orbit averaging to take advantage of disparate time scales and to improve further the computational efficiency of the simulation methods. This has been illustrated in two examples, a simple electrostatic model and an electrostatic gyrokinetic model. Furthermore, we have demonstrated in linear dispersion analyses that the highest-frequency, electron normal modes are rendered stable at large timestep in all three of the semi-implicit algorithms presented here. We will report simulation experience with these new methods in a future publication.

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Note added in proof. Since this paper was submitted and revised, implementation of the semi-implicit, orbit-averaged, electrostatic gyrokinetic algorithm has been undertaken. For applications in which quasi-neutrality is important and a high degree of cancellation should occur between the electron and ion charge densities, the time difference of the ion density on the right sides of Eqs. (9) and (19) should be replaced by $-4\pi \Delta T \nabla \cdot \mathbf{J}_{N+1/2}^i$ in Eq. (9) and the corresponding gyroaveraged form in Eq. (19) so that the ion and electron source terms in Poisson's equation are treated on a more equal footing with respect to finite-differencing effects. These changes have no influence on the numerical dispersion relations that are presented in this paper, which remain valid for $m_e \ll m_i$.

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