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An implicit δf particle-in-cell method with sub-cycling and orbit averaging for Lorentz ions

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ABSTRACT

A second order implicit δf Lorentz ion hybrid model with sub-cycling and orbit averaging has been developed to study low-frequency, quasi-neutral plasmas. Models using the full Lorentz force equations of motion for ions may be useful for verifying gyrokinetic ion simulation models in applications where higher order terms may be important. In the presence of a strong external magnetic field, previous Lorentz ion models are limited to simulating very short time scales due to the small time step required for resolving the ion gyromotion. Here, we use a simplified model for ion Landau damped ion acoustic waves in a uniform magnetic field as a test bed for developing efficient time stepping methods to be used with the Lorentz ion hybrid model. A detailed linear analysis of the model is derived to validate simulations and to examine the significance of ion Bernstein waves in the Lorentz ion model. Linear analysis of a gyrokinetic ion model is also performed, and excellent agreement with the dispersion results from the Lorentz ion model is demonstrated for the ion acoustic wave. The sub-cycling/orbit averaging algorithm is shown to produce accurate finite-Larmor-radius effects using large macro-time steps sizes, and numerical damping of high frequency fluctuations can be achieved by formulating the field model in terms of the perturbed flux density. Furthermore, a CPU–GPU implementation of the sub-cycling/orbit averaging is presented and is shown to achieve a significant speedup over an equivalent serial code.

1. Introduction

Modern research on low-frequency, ion-Larmor-radius scale fluctuations in magnetized plasmas is based on gyrokinetic ion models. One advantage for using gyrokinetic ion models, as opposed to models using the full Lorentz force equations of motion, is that the analytical elimination of the ion gyration time-scale in gyrokinetic models relaxes time step size constraints in numerical implementations. Additionally, gyrokinetic simulations accurately model $k_\perp \rho_i \sim O(1)$ effects without introducing noise associated with ion Bernstein waves, where $k_\perp$ is the wavenumber perpendicular to $\mathbf{B}$ and ρ_i is the ion gyroradius. Gyrokinetic theory, however, is based on a number of ordering assumptions which must hold to ensure the accuracy of the model. In certain applications where gyrokinetic ordering assumptions may be in questions, for example, in the tokamak edge pedestal region where gradient scale lengths can be comparable to the ion-Larmor-radius, higher order

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terms may be important. Extending gyrokinetic ion models for such applications, however, can be non-trivial and can lead to challenging numerical implementations [1–4].

There has been recent interest in developing models using the full Lorentz force equations of motion for ions [5–7]. Such models offer formal simplicity over gyrokinetic models and can provide an important validation tool or replacement for gyrokinetic ion models in applications where higher order terms may be important. Since time step size restrictions in simulation models which include kinetic electrons often require modern gyrokinetic codes to be run with time step sizes $\Omega_i \Delta t \sim 1$, the use of models which fully resolve the ion gyromotion may be feasible without a large increase in computational effort. Furthermore, recent efforts in optimizing particle-in-cell (PIC) algorithms for modern computing architectures, such as graphics processing units (GPUs), holds promise for handling the more expensive particle integration of the Lorentz ion model [8–11].

In this paper, we explore an implicit orbit averaging/sub-cycling (OASC) time stepping algorithm which may be useful for extending the ability of Lorentz force ion models to simulate longer time scales. This algorithm is shown to accurately produce finite-Larmor-radius (FLR) effects at perpendicular wave numbers $k_\perp \rho_i \sim O(1)$ while advancing the fields on a macro time step ΔT larger than that required to resolve the ion gyromotion. The accuracy of the ion gyromotion is preserved by sub-cycling the computational particles on a micro time step Δt chosen such that $\Omega_i \Delta t \ll 1$. The algorithm is applied to a model problem for ion Landau damped ion acoustic waves in a magnetized plasma. This model problem may be easily extended to model the ion temperature gradient (ITG) instability in slab geometry as in [7]. Linear theory for the model is derived to validate simulation results. Comparisons are also made with a linear dispersion relation obtained from the analysis of a gyrokinetic ion model. The dispersion results show very good agreement between the two models for the low frequency ion acoustic wave.

A notable effect in simulations using Lorentz force ions is the introduction of ion Bernstein waves near harmonics of the ion gyro-frequency [12,13]. These are electrostatic normal modes, which are analytically eliminated in gyrokinetic models, but are present when full ion dynamics are included. Linear theory based on the Laplace transform method is presented to determine the amplitudes of the normal modes relative to the initial perturbation size. The theory predicts ion Bernstein wave amplitudes which are comparable to the ion acoustic wave amplitude. Since the ion Bernstein waves are not damped, their presence in simulations may be undesirable for studies of low-frequency fluctuations. It is demonstrated that formulating the electrostatic field equation in terms of the ion particle flux density results in numerical damping for the ion Bernstein waves.

This paper is organized as follows. In Section 2, our model problem for ion Landau damped ion acoustic waves in a magnetized plasma is presented. Section 3 gives the linear theory for the model problem, including an analysis to derive information on the amplitudes of the normal modes. Section 4 gives the numerical methods used in our simulation model. In Section 5, simulation results are presented to demonstrate the numerical propertied of the implicit OASC algorithm and the accurate production of FLR effects at large macro time step sizes. Here, a comparison with the gyrokinetic ion model is also presented. A hybrid CPU–GPU implementation of our simulation model is discussed in Section 6 and is shown to achieve a speedup factor of ~ 48 compared to an equivalent serial CPU implementation. Section 7 contains further discussion and a summary.

2. Kinetic model for magnetized ion acoustic waves

Here we introduce the equations for the ion Landau damped ion acoustic wave model. We consider a uniform equilibrium distribution $\nabla f_0 = 0$ in a straight, uniform magnetic field $\mathbf{B} = B_0 \hat{z}$ and a self generated electrostatic field $\mathbf{E} = -\nabla\phi$, where ϕ is the electrostatic potential. The model is 2D-3V, meaning it is defined over two spatial dimensions and three velocity dimensions. The spatial dependence of quantities is over the two dimensional domain $(y, z) \in [0, L_\perp) \times [0, L_\parallel)$ and periodicity is assumed in both y and z outside the domain with periods $L_\perp$ and $L_\parallel$ respectively. The velocity dependence of quantities is over $(v_x, v_y, v_z) \in \mathbb{R}^3$. The ion distribution function f_i is taken to follow the Vlasov equation:

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla f_i + \frac{q_i}{m_i} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_i = 0, \tag{1}$$

where q_i and m_i are the ion charge and mass respectively. The electrons are assumed to be adiabatic, with number density n_e following:

$$n_e = n_0 \left(1 + \frac{e\phi}{T_e}\right), \tag{2}$$

where n_0 is the equilibrium density, e is the electron charge, and T_e is the electron temperature. Finally, quasi-neutrality is assumed:

$$n \equiv n_e = n_i = \int_{\mathbb{R}^3} f_i d\mathbf{v}. \tag{3}$$

Equations (1)–(3), along with the periodicity assumptions form a closed model. In particular, Eq. (1) can be solved for the ion distribution function f_i, Eq. (3) then used to provide an electron number density n_e, and finally Eq. (2) provides a way