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Nonlinear perturbative electromagnetic (Darwin) particle simulation of high intensity beams

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Abstract

A multi-species perturbative nonlinear (δf) electromagnetic particle simulation scheme has been developed for studying the propagation of intense charged particle beams in high-intensity accelerators and transport systems. The scheme is based on the Darwin approximation of Ampere's law, in which the transverse inductive electric field is neglected, resulting in the elimination of high-frequency transverse electromagnetic effects and, consequently, the associated numerical restrictions from the simulation. However, as noted previously, the presence of the time derivative of the vector potential in the equations of motion for the Darwin model can cause numerical instability. To circumvent this difficulty, we have adopted an approach by replacing the mechanical momentum, p_z, in the direction of beam propagation, by the canonical momentum, $P_z = p_z + qA_z/c$, as the phase-space variable. The resulting Ampere's law is then modified by the presence of an additional shielding term associated with the skin depth of the species. In order to minimize the numerical noise and to easily access both linear and nonlinear regimes for the physics of interest, we have also adopted the δf formalism for the Darwin model. The absence of unwanted high-frequency waves also enables us to use the adiabatic particle pushing scheme to compensate for the mass-ratio disparities for the various species of charge. The scheme is ideal for studying two-stream and filamentation instabilities, which may cause deterioration of the beam quality in the heavy ion fusion driver and fusion chamber. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

A multi-species perturbative nonlinear (δf) electromagnetic particle simulation scheme has been developed for studying the propagation of intense charged particle beams in high-intensity accelerators and transport systems for heavy ion fusion applications. The scheme is based on the Darwin approximation of Ampere's law, in which the transverse inductive electric field is neglected, resulting in the elimination of light waves as well as the associated numerical restrictions from the simulation. However, as noted in the past [1], the presence of the time derivative of the vector potential, $\partial \mathbf{A}/\partial t$, in the equations of motion for the Darwin model can cause numerical instabilities. To circumvent the difficulty, procedures involving the removal of $\partial \mathbf{A}/\partial t$ in the equations of motion have been developed, and the Darwin model have been successfully used in particle simulations for studying electromagnetic perturbations in plasmas, such as Weibel instabilities [1,2], whistler and magnetosonic waves [3] and shear

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Alfven waves [4]. Other methods involving the calculation of transverse inductive electric field have also been developed [5,6] In this paper, we adopted a procedure similar to the Hamiltonian formulation suggested by Nielson and Lewis [1] in which the mechanical momentum, $\mathbf{p} = m\mathbf{v}$, is replaced by the canonical momentum, $\mathbf{P} = \mathbf{p} + (q/c)\mathbf{A}$, as a phase-space variable so as to eliminate the troublesome $\partial\mathbf{A}/\partial t$ term, where q is the charge, c is the speed of light, and m is the mass. (The advantage of using the canonical momentum has long been recognized in magnetic fusion research for test particle transport [7] and for gyrokinetics [8,9].) In order to take advantage of the recent developments in perturbative particle simulations [10,11], the present scheme is also cast into the $\delta f(\equiv F - F_0)$ formalism, where F is the distribution function in phase space, and F_0 is the equilibrium distribution. As a result, the simulation plasma has minimal numerical noise, and also provides the ability to easily access both linear and nonlinear regimes for the physics of interest. Since the high-frequency waves associated with radiation fields are absent from the simulation, we can use the scheme of adiabatic particle pushing [12], for which the electrons are pushed more often, and with smaller time steps, than those for the ions and field equations so as to compensate for the mass ratio disparities for the different charge species. The scheme is ideal for studying two-stream [12] and filamentation [13] instabilities, which may cause deterioration of the beam quality in the heavy ion fusion driver and fusion chamber.

2. Overview of the Darwin model

The nonradiative limit of Maxwell's equations was first studied by Darwin [14] by neglecting the transverse part of the induction electric field in Ampere's law. The so-called Darwin model is valid to order $(v/c)^2$ and is very useful for studying electrostatic, magnetostatic and self-inductive electromagnetic effects in plasma and beam physics.

In terms of longitudinal (L) and transverse (T) quantities relative to the direction of wave propagation, the reduced Maxwell's equations for the Darwin model can be expressed as

$$\nabla \cdot \mathbf{E}^{\mathrm{L}} = 4\pi\rho, \tag{1}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J}^{\mathrm{T}}, \tag{2}$$

$$\frac{4\pi}{c}\mathbf{J}^{\mathrm{L}} + \frac{1}{c}\frac{\partial \mathbf{E}^{\mathrm{L}}}{\partial t} = 0, \tag{3}$$

and

$$\nabla \times \mathbf{E}^{\mathrm{T}} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \tag{4}$$

for which $\mathbf{E} = \mathbf{E}^{\mathrm{L}} + \mathbf{E}^{\mathrm{T}}$, $\nabla \times \mathbf{E}^{\mathrm{L}} = 0$, $\nabla \cdot \mathbf{E}^{\mathrm{T}} = 0$, $\nabla \cdot \mathbf{B} = 0$, $\mathbf{J} = \mathbf{J}^{\mathrm{L}} + \mathbf{J}^{\mathrm{T}}$, $\nabla \times \mathbf{J}^{\mathrm{L}} = 0$, and $\nabla \cdot \mathbf{J}^{\mathrm{T}} = 0$. Using the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, for

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{5}$$

we obtain Ampere's law expressed as

$$\nabla^2\mathbf{A} = -\frac{4\pi}{c}\mathbf{J}^{\mathrm{T}}, \tag{6}$$

and the induction (transverse) electric field can be obtained from

$$\mathbf{E}^{\mathrm{T}} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \tag{7}$$

or

$$\nabla^2\mathbf{E}^{\mathrm{T}} = \frac{4\pi}{c^2}\frac{\partial \mathbf{J}^{\mathrm{T}}}{\partial t}. \tag{8}$$

The longitudinal electric field is

$$\mathbf{E}^{\mathrm{L}} = -\nabla\Phi, \tag{9}$$

and the electrostatic potential is determined from Poisson's equation

$$\nabla^2\Phi = -4\pi\rho. \tag{10}$$

Moreover,

$$\mathbf{J}^{\mathrm{T}} = \mathbf{J} + \frac{1}{4\pi}\frac{\partial \mathbf{E}^{\mathrm{L}}}{\partial t}. \tag{11}$$

The numerical difficulty in applying the Darwin model is the use of the transverse electric field to push particles. To illustrate this point, let us use the magnetized, nonrelativistic Vlasov equation of the form,

$$\frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\left(\mathbf{E}^{\mathrm{L}} + \mathbf{E}^{\mathrm{T}} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\frac{\partial F}{\partial \mathbf{v}} = 0, \tag{12}$$

where the equations of motion for the particles are given by

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \tag{13}$$

and

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\left(\mathbf{E}^{\mathrm{L}} + \mathbf{E}^{\mathrm{T}} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right). \tag{14}$$

Since $\mathbf{E}^{\mathrm{T}} = -(1/c)\partial\mathbf{A}/\partial t$, the time advance of $\mathbf{v}$ cannot be time-centered, and numerical instabilities have been observed [1]. To circum-vent this problem, one can modify the way for calculating $\mathbf{E}^{\mathrm{T}}$. From Eq. (12), we first obtain

$$\frac{\partial\mathbf{J}}{\partial t} = -\frac{\partial}{\partial\mathbf{x}}\cdot q\int \mathbf{v}\mathbf{v}F\,\mathrm{d}\mathbf{v} + \frac{q^2}{m}\int\left(\mathbf{E}^{\mathrm{L}} + \mathbf{E}^{\mathrm{T}} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)F\,\mathrm{d}\mathbf{v}. \tag{15}$$

The transverse part of $\mathbf{J}$ can then be evaluated from Eq. (11), which, in turn, enables us to calculate $\mathbf{E}^{\mathrm{T}}$ directly from Eq. (8), without resorting to Eqs. (6) and (7). To avoid calculat-ing $\partial\mathbf{E}^{\mathrm{L}}/\partial t$ in Eq. (11), we can evaluate $\mathbf{J}^{\mathrm{T}}$ directly in Fourier $\mathbf{k}$ space by using the ansatz of $\exp(i\mathbf{k}\cdot\mathbf{x})$ and obtain transverse part of the current as

$$\mathbf{J}^{\mathrm{T}} = \mathbf{J} - (\mathbf{k}\cdot\mathbf{J})\,\mathbf{k}/k^2.$$

Busnardo-Neto et al. [3] has found this scheme to be numerically stable and used it for studying whistler and magnetosonic waves. However, it is evident that the scheme is rather cumbersome to implement.

3. Darwin model for relativistic beams

Here, we take a totally different approach by eliminating the time derivative of the transverse electric field in the equation of motion for the particles through the use of canonical momentum. The relativistic form of the Vlasov equation, Eq. (12), describing the propagation of an intense particle beam with narrow momentum spread through a smooth focusing external field can be expressed as [12]

$$\frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial\mathbf{x}} + \left[-\gamma m\omega_\beta^2\mathbf{x}_\perp + q\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\right] \times\frac{\partial F}{\partial\mathbf{p}} = 0, \tag{16}$$

where $\mathbf{v} = \mathbf{p}/\gamma m$, $\gamma = 1/\sqrt{1-\beta^2}$, and $\beta = \langle v_z\rangle/c$, z is the direction of beam propagation, $\langle v_z\rangle$ is the average axial velocity, $\mathbf{x}_\perp$ are the perpendicular displacement, and $\omega_\beta = \text{const.}$ is the effective applied betatron frequency for transverse (perpendicular) oscillations. For $\mathbf{J}_\perp \approx 0$, and $|\partial/\partial z| \ll |\partial/\partial\mathbf{x}_\perp|$, i.e., $k_\parallel \ll k_\perp$, Eq. (16) yields $J_z^{\mathrm{T}} \approx J_z$, and Ampere's law is simplified to become

$$\nabla_\perp^2 A_z = -\frac{4\pi}{c}J_z, \tag{17}$$

which gives

$$\mathbf{B} = \nabla\times A_z\hat{\mathbf{e}}_z \tag{18}$$

and

$$\mathbf{E}^{\mathrm{T}} = E_z^{\mathrm{T}}\hat{\mathbf{e}}_z = -\frac{1}{c}\frac{\partial A_z}{\partial t}\hat{\mathbf{e}}_z, \tag{19}$$

while Eq. (10) remains unchanged. The nonlinear Vlasov equation becomes

$$\frac{\partial F}{\partial t} + \mathbf{v}_\perp\cdot\frac{\partial F}{\partial\mathbf{x}_\perp} + v_z\frac{\partial F}{\partial z} - \left[\gamma m\omega_\beta^2\mathbf{x}_\perp + q\nabla_\perp\left(\Phi - \frac{v_z}{c}A_z\right)\right]\cdot\frac{\partial F}{\partial\mathbf{p}_\perp} - q\left(\frac{\partial\Phi}{\partial z} + \frac{1}{c}\frac{\partial A_z}{\partial t}\right)\frac{\partial F}{\partial p_z} = 0. \tag{20}$$

The troublesome term $\partial A_z/\partial t$ associated with orbit characteristics

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{p_z}{\gamma m} \tag{21}$$

and

$$\frac{\mathrm{d}p_z}{\mathrm{d}t} = -q\left(\frac{\partial\Phi}{\partial z} + \frac{1}{c}\frac{\partial A_z}{\partial t}\right) \tag{22}$$

can be eliminated by introducing

$$P_z = p_z + \frac{q}{c}A_z, \tag{23}$$

where P_z is the canonical momentum. From $\mathrm{d}A_z/\mathrm{d}t \approx \partial A_z/\partial t + v_z\partial A_z/\partial z$, we can re-write

these orbit characteristics as

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{1}{\gamma m}\left(P_z - \frac{q}{c}A_z\right), \tag{24}$$

and

$$\frac{\mathrm{d}P_z}{\mathrm{d}t} = -q\frac{\partial}{\partial z}\left(\Phi - \frac{v_z}{c}A_z\right). \tag{25}$$

Thus, by transforming from p_z to P_z, the time derivative of A_z conveniently disappears from the equations of motion. Together with

$$\frac{\mathrm{d}\mathbf{x}_\perp}{\mathrm{d}t} = \frac{\mathbf{p}_\perp}{\gamma m} \tag{26}$$

and

$$\frac{\mathrm{d}\mathbf{p}_\perp}{\mathrm{d}t} = -\gamma m\omega_\beta^2\mathbf{x}_\perp - q\nabla_\perp\left(\Phi - \frac{v_z}{c}A_z\right), \tag{27}$$

the Vlasov equation in the new coordinates can be written as

$$\frac{\mathrm{d}F}{\mathrm{d}t} \equiv \frac{\partial F}{\partial t} + \frac{\mathrm{d}\mathbf{x}_\perp}{\mathrm{d}t}\cdot\frac{\partial F}{\partial \mathbf{x}_\perp} + \frac{\mathrm{d}z\partial F}{\mathrm{d}t\,\partial z} + \frac{\mathrm{d}\mathbf{p}_\perp}{\mathrm{d}t}\cdot\frac{\partial F}{\partial \mathbf{p}_\perp} + \frac{\mathrm{d}P_z}{\mathrm{d}t}\frac{\partial F}{\partial P_z} = 0, \tag{28}$$

where the characteristics are defined by Eqs. (24)–(27). The corresponding δf formalism [10,11] can be derived by letting $F = F_0 + \delta f$, $\Phi = \Phi_0 + \delta\Phi$ and $A_z = A_{z0} + \delta A_z$, where F_0 satisfies

$$\frac{\partial F_0}{\partial t} + \frac{\mathrm{d}\mathbf{x}_\perp}{\mathrm{d}t}\cdot\frac{\partial F_0}{\partial \mathbf{x}_\perp} + \frac{\mathrm{d}z\partial F_0}{\mathrm{d}t\,\partial z} + \left.\frac{\mathrm{d}\mathbf{p}_\perp}{\mathrm{d}t}\right|_0\cdot\frac{\partial F_0}{\partial \mathbf{p}_\perp} + \left.\frac{\mathrm{d}P_z}{\mathrm{d}t}\right|_0\frac{\partial F_0}{\partial P_z} = 0,$$

and $|_0$ denotes the zeroth-order trajectories calculated from Eqs. (25) and (27) using the equilibrium fields, Φ_0 and A_{z0}. The perturbed distribution is determined from

$$\frac{\mathrm{d}\delta f}{\mathrm{d}t} = -\left.\frac{\mathrm{d}\mathbf{v}_\perp}{\mathrm{d}t}\right|_\delta\cdot\frac{\partial F_0}{\mathrm{d}\mathbf{v}_\perp} - \left.\frac{\mathrm{d}P_z}{\mathrm{d}t}\right|_\delta\frac{\partial F_0}{\partial P_z}, \tag{29}$$

where $|_\delta$ denotes the perturbed trajectories obtained from Eqs. (25) and (27) using the perturbed fields, $\delta\Phi$ and δA_z. Letting $W = \delta f/F$, the weight equation becomes

$$\frac{\mathrm{d}W}{\mathrm{d}t} = (1 - W)\frac{1}{F_0}\frac{\mathrm{d}\delta f}{\mathrm{d}t}. \tag{30}$$

In the Klimontovich–Dupree representation, the perturbed distribution is related to the particle weight through

$$\delta f = \sum_{j=1}^{N} W_j\delta(\mathbf{x}_\perp - \mathbf{x}_{\perp j})\delta(z - z_j)\delta(\mathbf{p}_\perp - \mathbf{p}_{\perp j}) \times \delta(P_z - P_{zj}), \tag{31}$$

where N is the total number of particles in the simulation. The time evolution of z_j, P_{zj}, $\mathbf{x}_{\perp j}$, $\mathbf{p}_{\perp j}$, and W_j for the jth particle are described by Eqs. (24)–(27), and (30), respectively. The corresponding Poisson's equation is

$$\nabla_\perp^2\Phi = -4\pi\sum_\alpha q_\alpha\int F_\alpha\,\mathrm{d}\mathbf{p}_\perp\,\mathrm{d}P_z, \tag{32}$$

and Ampere's law is

$$\left(\nabla_\perp^2 - \sum_\alpha\frac{\omega_{p\alpha}^2}{c^2}\right)A_z = -\frac{4\pi}{c}\sum_\alpha q_\alpha\int\frac{P_z}{\gamma_\alpha m_\alpha}F_\alpha\,\mathrm{d}\mathbf{p}_\perp\,\mathrm{d}P_z, \tag{33}$$

where α denotes charge species, $\omega_{p\alpha} \equiv \sqrt{4\pi n_\alpha e^2/m_\alpha}$ is the plasma frequency, and $n_\alpha = \int F_\alpha\,\mathrm{d}\mathbf{p}_\perp\,\mathrm{d}P_z$ is the number density. Thus, the zeroth-order fields, Φ_0 and A_{z0}, are obtained by using $F_{0\alpha}$ in these equations and the perturbed fields, $\delta\Phi$ and δA_z, by using δf_α.

4. Discussions

The Darwin simulation methodology described in this paper is most suitable for studying multi-species beams, when non-radiative electromagnetic effects are important, and it can easily be implemented in our existing 3D BEST code [12]. The numerical consequence of the skin depth term in Eq. (33), in addition to the Debye shielding term, will be explored. The use of the Darwin model for the investigation of the electron-ion two-stream instability [12] including the induction electric field will be reported in a subsequent paper.

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