3D MULTISPECIES NONLINEAR PERTURBATIVE PARTICLE SIMULATION OF INTENSE PARTICLE BEAMS

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Abstract

The Beam Equilibrium Stability and Transport (BEST) code, a 3D multispecies nonlinear perturbative particle simulation code, has been developed to study collective effects in intense charged particle beams described self-consistently by the Vlasov-Maxwell equations. This code provides an effective numerical tool to investigate collective instabilities, periodically-focused beam propagation in in alternating-gradient focusing fields, halo formation, and other important nonlinear process in intense beam propagation.

1 INTRODUCTION AND THEORETICAL MODEL

For accelerator applications to spallation neutron sources, tritium production, and heavy ion fusion, space-charge effects on beam equilibrium, stability, and transport properties become increasingly important. To understand these collective process at high beam intensity, it is necessary to treat the nonlinear beam dynamics self-consistently using the nonlinear Vlasov-Maxwell equations[1, 2, 3]. Recently, the δf formalism, a low-noise, nonlinear perturbative particle simulation technique, has been developed for intense beam applications, and applied to matched-beam propagation in a periodic focusing field[4, 5, 6, 7, 8] and other related problems. This paper reports recent advances in applying the δf formalism to simulate the nonlinear dynamics of an intense beam. The BEST code described here is a 3D multispecies nonlinear perturbative particle simulation code, which can be applied to a wide range of important collective processes in intense beams, such as the electron-ion two-stream instability[9, 10], periodically-focused beam propagation[11, 12], and halo formation. In the the theoretical model[9, 10, 13], we consider a thin, continuous, high-intensity ion beam ($j = b$), with characteristic radius r_b propagating in the z-direction through background electron and ion components ($j = e, i$), each of which is described by a distribution function $f_j(\boldsymbol{x}, \boldsymbol{p}, t)$. The charge components ($j = b, e, i$) propagate in the z-direction with characteristic axial momentum $\gamma_j m_j \beta_j c$, where $V_j = \beta_j c$ is the directed axial velocity, $\gamma_j = (1-\beta_j^2)^{-1/2}$ is the relativistic mass factor, e_j and m_j are the charge and rest mass, respectively, of a j-th species particle, and c is the speed of light in *vacuo*. For each component ($j = b, e, i$), the transverse and axial particle velocities in a frame of reference moving with axial velocity $\beta_j c\hat{\boldsymbol{e}}_z$ are assumed to be *nonrelativistic*. While the nonlinear δf formalism outlined here is readily adapted to the case of a *periodic* applied focusing force, for present purpose we make use of a *smooth-focusing* model in which the applied focusing force is described by

$$\boldsymbol{F}_j^{foc} = -\gamma_j m_j \omega_{\beta j}^2 \boldsymbol{x}_\perp, \tag{1}$$

where $\boldsymbol{x}_\perp = x\hat{\boldsymbol{e}}_x + y\hat{\boldsymbol{e}}_y$ is the transverse displacement, and $\omega_{\beta j} = const$ is the effective betatron frequency for transverse oscillation. For example, in the absence of background ions ($f_i = 0$), to describe the two-stream interaction between the beam ions ($j = b$) and background electrons ($j = e$), we normally assume $V_e = \beta_e c \simeq 0$. The space-charge intensity is allowed to be arbitrarily large, subject only to transverse confinement of the beam ions by the applied focusing force, and the background electrons are confined in the transverse plane by the space-charge potential $\phi(\boldsymbol{x}, t)$ due to the excess ion charge. In the electrostatic approximation, we represent the self-electric and self-magnetic fields by $\boldsymbol{E}^s = -\nabla\phi(\boldsymbol{x}, t)$ and $\boldsymbol{B}^s = \nabla \times A_z(\boldsymbol{x}, t)\hat{\boldsymbol{e}}_z$, respectively. For present purpose, assuming perturbations with long axial wavelength ($k_z^2 r_b^2 \ll 1$) and neglecting the perturbed axial force on the charge components, the nonlinear Vlasov-Maxwell equation in the five-dimensional phase space $(\boldsymbol{x}, \boldsymbol{p}_\perp)$ can be approximated by[9, 10, 13]

$$\begin{aligned}\Big\{\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\frac{\partial}{\partial \boldsymbol{x}} - [\gamma_j m_j \omega_{\beta j}^2 \boldsymbol{x}_\perp \\ + e_j \nabla_\perp(\phi - \beta_j A_z)]\cdot\frac{\partial}{\partial \boldsymbol{p}_\perp}\Big\} f_j(\boldsymbol{x}, \boldsymbol{p}_\perp, t) = 0,\end{aligned} \tag{2}$$

and

$$\begin{aligned}\nabla_\perp^2 \phi &= -4\pi \sum_j e_j \int d^2\boldsymbol{p} f_j(\boldsymbol{x}, \boldsymbol{p}_\perp, t), \\ \nabla_\perp^2 A_z &= -4\pi \sum_j e_j \beta_j \int d^2\boldsymbol{p} f_j(\boldsymbol{x}, \boldsymbol{p}_\perp, t).\end{aligned} \tag{3}$$

Here, $\nabla_\perp = \hat{\boldsymbol{e}}_x \partial/\partial x + \hat{\boldsymbol{e}}_y \partial/\partial y$ and $\boldsymbol{v} = V_j \hat{\boldsymbol{e}}_z + (\gamma_j m_j)^{-1}\boldsymbol{p}_\perp$.

2 NONLINEAR δF SIMULATION METHOD AND THE BEST CODE

In the nonlinear δf formalism, we express the total distribution function as $f_j = f_{j0} + \delta f_j$, where f_{j0} is a *known* solution to the nonlinear Vlasov-Maxwell equations (2) and

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(3), and determine the detailed evolution of the perturbed distribution function $\delta f_j \equiv f_j - f_{j0}$. This is accomplished by advancing the weight function defined by $w_j \equiv \delta f_j / f_j$, together with the particles' positions and momenta. The equations of motion for the particles, obtained from the characteristics of the nonlinear Vlasov equation (2), are given by

$$\begin{aligned} \frac{d\boldsymbol{x}_{ji}}{dt} &= V_j \hat{\boldsymbol{e}}_z + (\gamma_j m_j)^{-1} \boldsymbol{p}_{\perp ji}, \\ \frac{d\boldsymbol{p}_{\perp ji}}{dt} &= -\gamma_j m_j \omega_{\beta j}^2 \boldsymbol{x}_{\perp ji} - e_j \nabla_\perp (\phi - \beta_j A_z). \end{aligned} \tag{4}$$

Here the subscript "ji" labels the i-th simulation particle of the j-th species. The weight functions w_j, as functions of phase space variables, are carried by the simulation particles, and the dynamical equations for w_j are easily derived from the definition of w_j and the Vlasov equation (2). Following the algebra in Refs. [4, 5, 6, 7], we obtain

$$\begin{aligned} \frac{dw_{ji}}{dt} &= -(1 - w_{ji}) \frac{1}{f_{j0}} \frac{\partial f_{j0}}{\partial \boldsymbol{p}_\perp} \cdot \delta\Big(\frac{d\boldsymbol{p}_{\perp ji}}{dt}\Big), \\ \delta\Big(\frac{d\boldsymbol{p}_{\perp ji}}{dt}\Big) &\equiv \frac{d\boldsymbol{p}_{\perp ji}}{dt}\bigg|_{(\phi, A_z) \longrightarrow (\delta\phi, \delta A_z)}, \end{aligned} \tag{5}$$

where $\delta\phi = \phi - \phi_0$ and $\delta A_z = A_z - A_{z0}$. Here, the equilibrium solutions (ϕ_0, A_{z0}, f_{j0}) solve the steady-state ($\partial/\partial t = 0$) Vlasov-Maxwell equations (2) and (3) with $\partial/\partial z = 0$ and $\partial/\partial\theta = 0$. A wide variety of axisymmetric equilibrium solutions to Eqs. (2) and (3) have been investigated in the literature. The perturbed distribution δf_j is obtained through the weighted Klimontovich representation

$$\delta f_j = \frac{N_j}{N_{sj}} \sum_{i=1}^{N_{sj}} w_{ji} \delta(\boldsymbol{x} - \boldsymbol{x}_{ji}) \delta(\boldsymbol{p}_\perp - \boldsymbol{p}_{\perp ji}), \tag{6}$$

where N_j is the total number of actual j-th species particles, and N_{sj} is the total number of *simulation* particles for the j-th species. Maxwell's equations are also expressed in terms of the perturbed fields and perturbed density according to

$$\begin{aligned} \nabla_\perp^2 \delta\phi &= -4\pi \sum_j e_j \delta n_j, \\ \nabla_\perp^2 \delta A_z &= -4\pi \sum_j e_j \beta_j \delta n_j, \\ \delta n_j &= \int d^2\boldsymbol{p}\, \delta f_j(\boldsymbol{x}, \boldsymbol{p}_\perp, t) = \frac{N_j}{N_{sj}} \sum_{i=1}^{N_{sj}} w_{ji} U(\boldsymbol{x}, \boldsymbol{x}_{ij}). \end{aligned} \tag{7}$$

Here, $U(\boldsymbol{x}, \boldsymbol{x}_{ij})$ represents the method of distributing particles on the grids in configuration space. The nonlinear particle simulations are carried out by iteratively advancing the particle motions, including the weights they carry, according to Eqs. (4) and (5), and updating the fields by solving the perturbed Maxwell's equations (7) with appropriate boundary conditions at the cylindrical conducting wall. Even though it is a perturbative approach, the δf method is fully nonlinear and simulates the original nonlinear Vlasov-Maxwell equations. Compared with conventional particle-in-cell simulations, the noise level in δf simulations is significantly reduced. In addition, the δf method can be used to study *linear* stability properties provided the factor $(1 - w_{ji})$ in Eq. (5) is approximated by 1, and the forcing term in Eq. (4) is replaced by the unperturbed force (i.e., advancing particles along the unperturbed orbits). Implementation of the 3D multispecies nonlinear δf simulation method described above is embodied in the BEST code at the Princeton Plasma Physics Laboratory. The code advances the particle motions using a 4th-order Runge-Kutte method, and solves Maxwell's equations by a fast Fourier transform and finite-difference method in cylindrical geometry. Written in Fortran 90/95, the code utilizes extensively the object-oriented features provided by the computer language. The NetCDF scientific data format is implemented for large-scale diagnostics and visualization. The code has achieved an average speed of 40μs/(particle$\times$step) on a DEC alpha personal workstation 500au computer.

3 SIMULATION RESULTS

For brevity, we present here illustrative simulation results for a single-species thermal equilibrium ion beam in a constant focusing field. In this case, equilibrium properties depend on the radial coordinate $r = (x^2 + y^2)^{1/2}$. The thermal equilibrium distribution function is given by

$$\begin{aligned} f_{b0}(r, \boldsymbol{p}_\perp) &= \frac{\hat{n}_b}{2\pi\gamma_b m_b T_b} \\ &\times \exp\Big\{-\frac{p_\perp^2/2\gamma_b m_b + \gamma_b m_b \omega_{\beta b}^2 r^2/2 + e_b(\phi_0 - \beta_b A_{z0})}{T_b}\Big\} \end{aligned} \tag{8}$$

where $\hat{n}_b$ is the density of beam particles at $r = 0$, and T_b is the transverse temperature of the beam ions in energy units. It is also assumed that the beam is centered inside a cylindrical chamber with perfectly conducting wall located at $r = r_w$. The equilibrium self-field potentials ϕ_0 and A_{z0} can be determined numerically from Maxwell's equations (3). First, we examine the nonlinear propagation properties of the beam. A random initial perturbation is introduced into the system, and the beam is propagated from $t = 0$ to $t = 500\tau_\beta$, where $\tau_\beta \equiv \omega_{\beta b}^{-1}$. The simulation results show that the perturbations do not grow and the beam propagates quiescently, which agrees with the nonlinear stability theorem[14, 15] for the choice of equilibrium distribution function in Eq. (8). Shown in Fig. 1 is a plot of the change in transverse emittance-squared (normalized by $V_b^2/\omega_{\beta b}^2$), $\delta\epsilon^2 = \epsilon^2(t) - \epsilon_0^2$, versus normalized time t/τ_β, for perturbations about the thermal equilibrium distribution in Eq. (8). The system parameters in Fig. 1 correspond to protons with $\gamma_b = 1.85$, and normalized beam intensity $K\beta_b c\tau_\beta/\epsilon_0 = 0.025$, where $K = 2N_b e^2/\gamma_b^3 m_b \beta_b^2 c^2$ is the self-field perveance, and N_b is the number of beam ions per unit axial length. The amplitudes of the initial random perturbation in weights in Fig. 1 is 10^{-4}, which leads to the very small offset in $\delta\epsilon^2$. It is evident from Fig. 1 that the variations in beam emittance, $\delta\epsilon^2$, remain extremely small for perturbations about a thermal equilibrium beam. As a

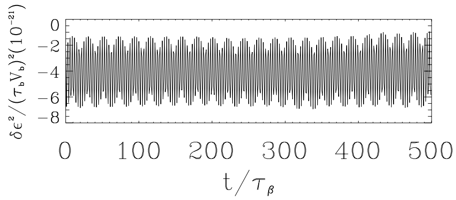

Figure 1: Plot of $\delta\epsilon^2$ versus t/τ_β

second example, we study the linear surface mode for perturbations about a thermal equilibrium beam in the space-charge-dominated regime, with flat-top density profile and $K\beta_b c\tau_\beta/\epsilon_0 \gg 1$. These modes are of practical interest because they can be destabilized by a two-stream electron-ion interaction when background electrons are present[9, 10]. The BEST code, operating in its linear stability mode, has recovered very well-defined eigenmodes with mode structures and eigenfrequencies which agree well with theoretical predications. For $K\beta_b c\tau_\beta/\epsilon_0 \gg 1$, and azimuthal mode number $l = 1$, the dispersion relation for these modes is given by[1, 9, 10]

$$\omega = k_z V_b \pm \frac{\hat{\omega}_{pb}}{\sqrt{2}\gamma_b}\sqrt{1 - \frac{r_b^2}{r_w^2}}, \tag{9}$$

where r_b is the radius of the beam edge, and r_w is location of the conducting wall. In Eq. (9), $\hat{\omega}_{pb}^2 = 4\pi\hat{n}_b e_b^2/\gamma_b m_b$ is the ion plasma frequency-squared, and $\hat{\omega}_{pb}/\sqrt{2}\gamma_b \simeq \omega_{\beta b}$ in the space-charge-dominated limit. Shown in Fig. 2 is the comparison between plots of the eigenfrequency versus r_w/r_b obtained from the simulations (diamonds and triangles) and that predicted by Eq. (9) (solid curves). The parameters for this case are chosen close to the space-charge limit with $K\beta_b c\tau_\beta/\epsilon_0 = 6.59$, and the perturbation has normalized axial wavenumber $k_z V_b/\omega_{\beta b} = 2\pi$. It is clear from Fig. 2 that the simulation results agree well with theory.

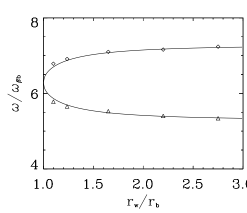

Figure 2: Eigenfrequency versus r_w/r_b.

4 CONCLUSION AND FUTURE WORK

The BEST code has been tested and applied in different scenarios. As a 3D multispecies perturbative particle simulation code, it provides several unique capabilities. Since the simulation particles are used to simulate only the perturbed distribution function and self-fields, the simulation noise is reduced significantly. The perturbative approach also enables the code to investigate different physics effects separately, as well as simultaneously. The code can be easily switched between linear and nonlinear operation, and used to study both linear stability properties and nonlinear beam dynamics. These features, combined with 3D and multispecies capabilities, provide us with an effective tool to investigate the electron-ion two-stream instability, periodically focused solutions in alternating focusing fields, halo formation, and many other important problems in nonlinear beam dynamics and accelerator physics. Finally, the BEST code is readily adapted to the case where the applied focusing force, $\boldsymbol{F}_j^{foc}$, corresponds to a periodic focusing quadrapole field or solenoidal field, and the effects of the axial self-field field $\boldsymbol{F}_{jz}^s = -\hat{\boldsymbol{e}}_z e_j \partial\phi(\boldsymbol{x}, t)/\partial z$ on the particle dynamics are retained self-consistently. Results of these studies will be reported in future publications.

5 ACKNOWLEDGMENT

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