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New Scheme for Electromagnetic Simulations

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A new explicit time stepping scheme for electromagnetic simulations is described, the *neo-finite-difference* method. This numerical method which describes the time derivative as an arc instead of a straight line is more accurate. Thus, larger time steps can be used than with the standard leapfrog method. We start by Fourier analyzing the electromagnetic field in space. The Fourier amplitudes obey harmonic oscillator equations in time. The method involves approximating the time advance of a mode's amplitude from oscillator solutions for its estimated frequencies. From a computational point of view this involves replacing Δt by $2\sin[\omega^E(k)\Delta t/2]/\omega^E(k)$ in the finite difference equations, where $\omega^E(k)$ is the estimated frequency of mode k; that is, Δt is multiplied by a k-dependent correction constant. The method not only improves the accuracy of the time stepping algorithm, but it increases the size of Δt for which it is stable. The ion-ripple laser is used as an example of a neo-finite difference electromagnetic simulation application to illustrate the new scheme. The size of the time step in the new scheme may be chosen one order of magnitude larger than for the standard method. The new scheme does not change the computation time per time step and only requires slight changes to the original code.

I. INTRODUCTION

The limitation on the size of time step for a standard electromagnetic simulation is either the Courant–Friedrichs–Lewy condition [1–6] for a simulation solving wave equations in finite spatial grids or the stability condition of ordinary differential equations in Fourier space. The size of the time step required not to violate the stability condition may be much smaller than that needed to resolve the time variation of physical quantities. This makes standard simulation slower.

There are some efforts toward trying to use a larger time step. Consider the case of a particle executing circular motion under an external longitudinal magnetic field. In order to have the correct gyrophase and gyroradius, correction constants have been added into the particle's equation of motion and the amplitude of its velocity [5, 7, 8]. This application is limited to gyromotion and is not related to the stability conditions. The other case is that of light waves propagating in a vacuum [9–11]. Light waves can be divided into left-going and right-going fields. They are advanced in time with the speed of light to assure a correct phase change. This is only applicable when the effect of the medium is not important and the directions of the wave propagation are well oriented.

We propose here a new scheme for electromagnetic simulations. This explicit scheme corrects the errors of the standard field solver and improves the accuracy and stability of the time integration procedure by employing our neo-finite-difference method, which can be applied to wide areas of numerical computation and will be published in a separate paper [15]. In this new scheme, a fast Fourier transform in space is used, and the standard leapfrog time integration is improved. In the next section, we explain the problem of the old field solver. Then, the new scheme is presented. In Section III, we test this new electromagnetic simulation scheme. The ion-ripple laser [14] is used as an example. The frequency error of electromagnetic waves in the old scheme is eliminated in the new scheme. The accuracy is greatly improved. So, the size of the time step for an electromagnetic simulation using the new scheme is no longer restricted by the usual stability condition. The size can be much larger. Section IV is the summary and discussion.

II. THEORY OF THE NEW ELECTROMAGNETIC SCHEME

We assume a periodic system and, hence, we can work in Fourier space. Electromagnetic waves interacting with a plasma are described by Maxwell's equations,

$$\frac{\partial \tilde{B}}{\partial t} = -ic\mathbf{k} \times \tilde{E}, \tag{1}$$

$$\frac{\partial \tilde{E}}{\partial t} = ic\mathbf{k} \times \tilde{B} - 4\pi \tilde{J}, \tag{2}$$

where $\tilde{E}(\tilde{B})$ are the electric (magnetic) fields of the waves, $\tilde{J}(\mathbf{k})$ is the plasma current responding to the wave, c is the speed of light, and we have assumed that the fields are of the Fourier form $(\mathbf{E}, \mathbf{B}, \mathbf{J}) = (\tilde{E}, \tilde{B}, \tilde{J})e^{i\mathbf{k}\cdot\mathbf{x}}$.

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If space charge effects are included, we also need Poisson equation,

$$\mathbf{k} \cdot \tilde{E} = 4\pi q n(\mathbf{k}), \tag{3}$$

where $n(\mathbf{k})$ is the charge density of mode $\mathbf{k}$, and q is the particle charge. To obtain the plasma response, we use the equation of particle motion,

$$\frac{d\mathbf{P}}{dt} = q\left(\mathbf{E} + \frac{\mathbf{v} \times \boldsymbol{B}}{c}\right), \tag{4}$$

where $\mathbf{P} = \gamma m_p \mathbf{v}$ is the particle momentum, m_p is the rest mass, $\gamma = (1 - |\mathbf{v}|^2/c^2)^{-1/2}$ is the Lorentz factor, $\mathbf{v}$ is the velocity, and $\mathbf{J}(x) = qn(x)\mathbf{v}$ is the current. Equations (1)–(4) are nonlinear so that analytic solutions for interesting nonlinear situations are rare. However, we may still be able to estimate fairly accurately the frequency of each $\mathbf{k}$ mode for the purpose of the new time-differencing method; this is particularly true for the large k modes that are most limiting for the time step size. By using the standard finite difference method, for a single wave, Eqs. (1) and (2) can be expressed as

$$\tilde{B}^{n+1/2} - \tilde{B}^{n-1/2} = -i\mathbf{k} \times \tilde{E}^n c\,\Delta t, \tag{5}$$

$$\tilde{E}^{n+1} - \tilde{E}^n = i\left[\mathbf{k} \times \tilde{B}^{n+1/2} + \frac{4\pi i}{c}\tilde{J}^{n+1/2}\right] c\,\Delta t, \tag{6}$$

where the leapfrog integration method is employed.

For a transverse wave ($\mathbf{k} \cdot \mathbf{E} = 0$), which can be Fourier analyzed in time (i.e., $(\mathbf{E}, \mathbf{B}, \mathbf{J}) = (\tilde{E}, \tilde{B}, \tilde{J})e^{-i\omega t}$), Eqs. (1) and (2) give

$$\omega^E = kc\frac{E}{B}, \tag{7}$$

$$E^2 = B^2 + \left|\frac{4\pi}{kc}\tilde{J} \cdot \tilde{B}^*\right|, \tag{8}$$

where ω^E is the correct wave frequency of Maxwell equations. Equations (7) and (8) are the exact dispersion relation and are determined by the plasma properties.

In the finite difference treatment, Eqs. (5) and (6) give

$$\sin\frac{\omega^s_{em}\Delta t}{2} = \frac{kc\,\Delta t}{2}\frac{E}{B} = \frac{kc\,\Delta t}{2}\frac{|\tilde{B} - (4\pi i/kc)\tilde{J}|}{E}, \tag{9}$$

or

$$\omega^s_{em} = \frac{2}{\Delta t}\sin^{-1}\frac{\omega^E\Delta t}{2}, \tag{10}$$

where ω^s_{em} is the wave frequency of mode k from the simulation

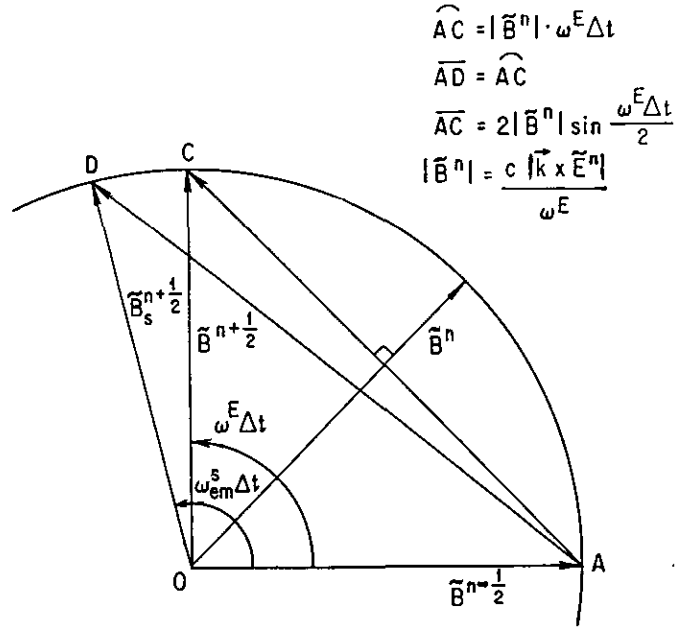

FIG. 1. The magnetic field is advanced by the new scheme (**AC**) and the old scheme (**AD**), respectively.

using the standard finite difference method, $E = |\tilde{E}|$, $B = |\tilde{B}|$, $J = |\tilde{J}|$, and $k = |\mathbf{k}|$. For a small time step (i.e., $\omega^E\,\Delta t \ll 1$), the numerical dispersion relation, Eq. (10), gives $\omega^s_{em} \sim \omega^E[1 + (\omega^E\,\Delta t)^2/24]$. The standard finite difference method not only makes an error on the wave frequency but it is also responsible for the stability condition. As indicated in Eq. (9), if $kc\,\Delta t/2 > \min\{B/E, E/|\tilde{B} - (4\pi i/kc)\tilde{J}|\}$, the wave frequency of simulation becomes a complex number. Thus, the wave fields grow exponentially. This numerical instability is due to the inaccuracy of the standard time-differencing. Although the system can become stable by truncating short wavelength modes and/or decreasing the size of time step, the frequency error is always there.

The problem with the old scheme can also be described by Fig. 1, which is in the phase plane for a linearly polarized wave and in the transverse spatial plane for a circularly polarized wave. The differential equation (e.g., Eq. (1)) follows the exact trajectory of an arc (i.e., $\widehat{AC}$), but the standard finite difference method follows a straight line. While the driving term (the right-hand side of Eq. (5)) gives an arc $\widehat{AC}$, the standard finite difference method (the left-hand side of Eq. (5)) advances the magnetic field to $\tilde{B}_s^{n+1/2}$ (**OD**) by a straight line $\overline{AD}$ whose length is equal to the arc length such that the phase advance is not correct. The wave frequency of the old scheme ω^s_{em} is greater than the correct frequency ω^E. We correct this error by using the neo-finite-difference method; that is,

$$\left[\frac{\omega^E\,\Delta t/2}{\sin(\omega^E\,\Delta t/2)}\right](\tilde{B}^{n+1/2} - \tilde{B}^{n-1/2}) = -i\mathbf{k} \times \tilde{E}^n c\,\Delta t, \tag{11}$$

$$\left[\frac{\omega^E \Delta t/2}{\sin(\omega^E \Delta t/2)}\right](\tilde{E}^{n+1} - \tilde{E}^n) = i\left[\mathbf{k} \times \tilde{B}^{n+1/2} + \frac{4\pi i}{c}\tilde{J}^{n+1/2}\right] c\,\Delta t, \tag{12}$$

where ω^E depends on the plasma property. The frequency can be calculated from Eqs. (7) at each time step or estimated by Eqs. (7) and (8) (the knowledge of the plasma property). Equation (11) (Eq. (12)) advances the magnetic field (the electric field) by an arc (i.e., $\widehat{AC}$). Equations (11) and (12) can also be expressed by

$$\tilde{B}^{n+1/2} - \tilde{B}^{n-1/2} = -i\mathbf{k} \times \tilde{E}^n\, c\,\Delta t\left[\frac{\sin(\omega^E \Delta t/2)}{\omega^E \Delta t/2}\right], \tag{13}$$

$$\tilde{E}^{n+1} - \tilde{E}^n = i\left[\mathbf{k} \times \tilde{B}^{n+1/2} + \frac{4\pi i}{c}\tilde{J}^{n+1/2}\right] c\,\Delta t\left[\frac{\sin(\omega^E \Delta t/2)}{\omega^E \Delta t/2}\right]. \tag{14}$$

Equations (13) and (14) make the difference term smaller (i.e., **AC**) and give the wave frequency of mode k,

$$\omega_{em} = \omega^E, \tag{15}$$

where the wave frequency is correct and shows the stability of the new scheme. This new field solver corrects the wave frequencies and, hence, phase errors. The accuracy is improved. Also, the size of the time step can be made much larger without numerical instability setting in. The limit on the size of the time step depends on the resolution of the electromagnetic wave frequency of interest and approximations made in calculating J. Larger time steps cause a decrease of resolution. If the estimated wave frequency is not accurate, an overestimated correction constant, $(\omega^E \Delta t)/2 \sin(\omega^E \Delta t/2)$, used in Eqs. (11) and (12) does not cause numerical instability, while an underestimated one may cause it, especially for $\omega^E \Delta t \sim (m + 1)\pi$, where m is an integer (aliasing).

Previous studies [5, 9, 10, 11] rotate the electric field and the magnetic field together for each mode, according to the phase change in a vacuum. Their electric and magnetic fields are at the same time step. Our method is a leapfrog one which makes it more accurate and it also includes dispersive effects of the plasma. The fields at pre-advanced steps and at advanced steps (e.g., E^n and E^{n+1} in Eq.(14), respectively) have the same (unit) coefficient but the earlier treatments do not (e.g., the coefficient for E^n in Eq. 15-9b (3a) of Ref. [5] is cos $ck\,\Delta t$ when E^{n+1} is unity, which induces error). Their method has also under estimated the correction constant needed. We note that in the limit of no plasma both methods are exact. However, plasma is always of concern and our scheme can be applied to that regime. Furthermore, the two methods are different in concept and our method is much more general. All we need to know for the new scheme is the linear dispersion of the waves in plasma, which can often be obtained from linear theory or from a short test run. In the next section we will discuss electromagnetic waves in an unmagnetized plasma, for which the dispersion relation is $\omega^E \sim (k^2c^2 + \omega_{pe}^2)^{1/2}$, where ω_{pe} is the plasma frequency.

The method is also being successfully applied to simulations of a multidimensional magnetized plasma with ions and electrons [13]. For any given k, the highest frequency mode of the plasma is the R-wave, followed by the X-wave. That treatment makes corrections to the field solver using the wave frequency estimated from their linear dispersion relation, evaluated for the each given value of k. Since this method follows the linearized solutions, the accuracy is greatly improved. Thus, we can increase our time step size about fivefold.

III. SIMULATION OF THE NEW ELECTROMAGNETIC SCHEME

We have imposed the new field solver on a periodic relativistic 1 2/2 D particle-in-cell simulation code [12]. This only needs to change two statements for the form factor in the time stepping for the fields by replacing Δt by $\Delta t \cdot \sin(\omega^E \Delta t/2)/(\omega^E \Delta t/2)$. The computation time per time step does not increase. This simulation code uses the improved leapfrog integration on temporal differences and the fast Fourier transform and subtracted dipole interpolation on spatial differences. A Gaussian shape is assigned for the simulation particles. A unit length is a grid size. Time is normalized to ω_{pe}^{-1}, where $\omega_{pe}^2 = (4\pi n_e e^2)/m_e$ is the plasma frequency, n_e is the electron density, and m_e is the electron mass.

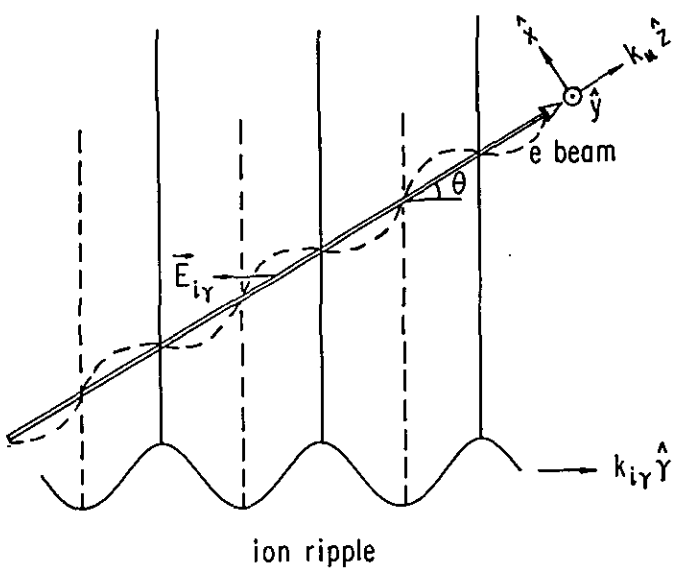

FIG. 2. An ion-ripple laser configuration.

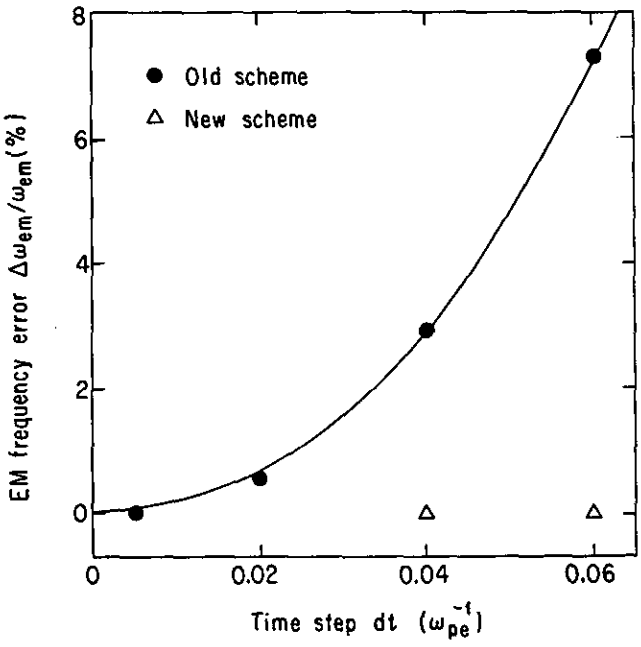

FIG. 3. Compare the frequency errors induced by the old scheme and the new scheme.

The physical problem chosen to test the code is the ion-ripple laser [14], which is a new concept to generate coherent tunable microwaves to X rays with the appropriate choice of parameters by using a relativistic electron beam obliquely passing through an ion ripple in plasma. The electric field of the ion ripple has a component transverse to the beam direction as shown in Fig. 2, where k_{ir} is the wave number of the ion ripple and $k_u = k_{ir} \cdot \cos\theta$. The transverse electric force causes the beam electrons to radiate. As the beam velocity, v_0, is much greater than the modulated transverse velocity v_x, the problem can be assumed to be one-dimensional. The dispersion relation has been derived [14] as

$$\varepsilon_{em}\varepsilon_{es} = C_f, \tag{16}$$

where

$$\varepsilon_{em} = \omega^2 - k^2c^2 - \omega_{pe}^2/\gamma_0, \tag{17}$$

$$\varepsilon_{es} = (\omega - k_p v_0)^2 - (\omega_{pe}^2 + 3k_p^2 v_t^2)/\gamma_0^3, \tag{18}$$

$$C_f = k^2 v_x^2 \omega_{pe}^2/4\gamma_0^3, \tag{19}$$

γ_0 is the beam's initial γ, $\gamma_0 \gg 1$, v_t is the thermal velocity of beam. Putting $\varepsilon_{em} = 0$ gives the dispersion relation for electromagnetic modes in a uniform plasma; $\varepsilon_{es} = 0$ is the dispersion relation for electrostatic modes for wave numbers $k_p = k + k_u$ (conservation of momentum) in a uniform plasma. C_f is the coupling factor for electromagnetic modes and electrostatic modes due to the ion ripple. The radiant wave frequency can be determined by their intersection; that is, $\omega_{em} = \omega_{es}$ (conservation of energy), where $\omega_{em} = (k^2c^2 + \omega_{pe}^2/\gamma_0)^{1/2}$ is the frequency of an electromagnetic mode, $\omega_{es} = k_p v_0 - S$ is the frequency of slow electrostatic beam mode, and $S = (\omega_{pe}^2 + 3k_p^2 v_t^2)^{1/2}/\gamma_0^{3/2}$. The coupling factor provides the source of instabilities and a small variation to the radiation frequency.

The physical parameters to be simulated are $\gamma_0 \sim 3$, $\theta = 45°$, $k_u c/\omega_{pe} = 1.6$, and $\varepsilon_i = 0.3$. The simulation system's parameters are the system length $L = 1024$, $c = 26$, the particle size $a = 0.6$, number of electron particles = 10,240, the ions do not move, and the Fourier modes that are kept ran from 0 to 256; this gives the maximum wave number $k_{max} = \pi/2$. The estimated wave frequencies to be used in the neo-finite-difference form factor of Eqs. (11) and (12) are taken to be $\omega^E = \omega_{em} = (k^2c^2 + \omega_{pe}^2/\gamma_0)^{1/2}$. We may also calculate the wave frequencies from Eqs. (7) at each time step. However, the formula of estimated wave frequencies that we use here is simple and only requires us to change two statements of the form factor of our existing simulation code. This change does not cost any computation time per time step because the iteration loop remains the same.

The simulation system is initialized in equilibrium. At $t = 0$, the total energy is TOT $\sim 3 \times 10^7$, the total electrostatic energy is TEL $\sim 6 \times 10^4$, the total electric energy of electromagnetic modes is TET $\sim 1 \times 10^5$, the total magnetic energy of electromagnetic modes is TEB $\sim 1 \times 10^3$, and the total kinetic energy is EXK $\sim 3 \times 10^7$. Using the standard leapfrog method and the size of time step $\Delta t = 0.06$ (i.e., $c\,\Delta t \sim 1.56$, which violates the Courant condition), we observed a very strong numerical instability. All energies grow exponentially.

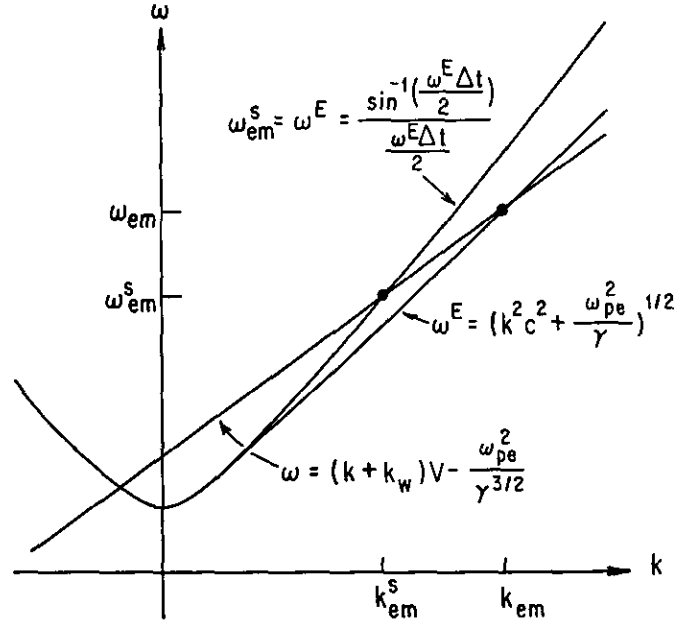

FIG. 4. The dispersion curves of slow electrostatic mode, exact electromagnetic mode, and old scheme simulation's electromagnetic mode.

At $t = 6$, TOT $\sim 6 \times 10^{108}$, TEL $\sim 2 \times 10^{6}$, TET $\sim 4 \times 10^{108}$, TEB $\sim 2 \times 10^{108}$, and EXK $\sim 1 \times 10^{56}$. As we apply the new scheme with the same size of time step, energy is quite well conserved. The error in total energy is within 0.1% after 5000 time steps.

Figure 3 is shown to compare the errors of an electromagnetic wave (mode 125 ($kc \sim 19.94$)) frequency induced by the standard finite difference scheme and neo-finite-difference scheme. The frequency error induced by the old scheme is as the prediction of Eq. (10). The new scheme with the neo-finite-difference method has almost eliminated the frequency error completely, such that it can make the size of time step much larger.

The frequency errors of simulation also produce incorrect physics results such as radiation spectrum. The radiation frequency of ion-ripple laser is near the intersection of the electromagnetic mode and the slow electrostatic mode. This is at (ω_{em}, k_{em}) of the dispersion diagram (ω, k) as shown in Fig. 4. But due to the errors of electromagnetic wave frequency induced by the standard time-differencing, the simulation of old scheme will move the interaction point to $(\omega^s_{em}, k^s_{em})$. The shift of radiation spectrum can be severe because the dispersion line of the electrostatic mode is very close to the dispersion curve of the electromagnetic mode, especially for a relativistic beam case. We show the shift of intersection points by the old scheme simulation in Fig. 5. The intersection points of the simulation are at

$$0 = \omega^s_{em} - \omega_{es} = (\omega^s_{em} - \omega_{em}) - (\omega_{es} - \omega_{em}) \qquad (20)$$

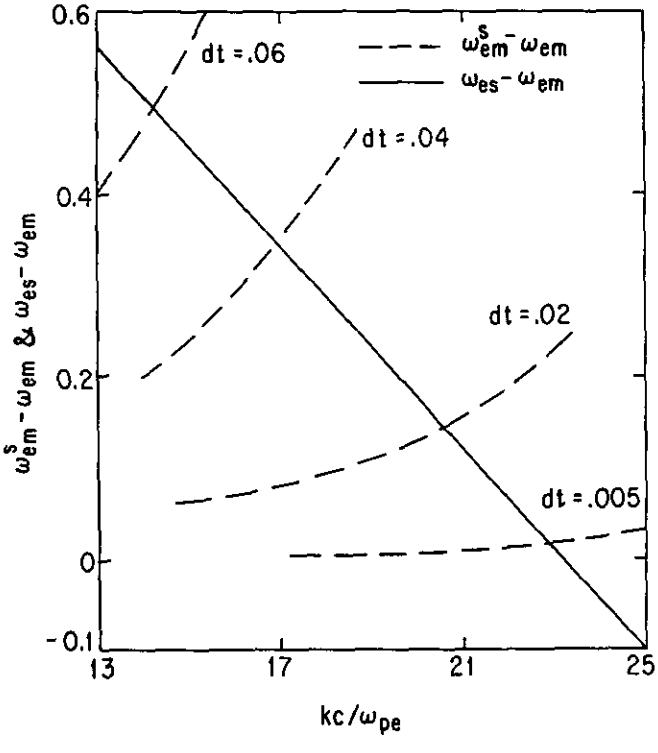

FIG. 5. The shifts of intersection points in the old scheme simulation.

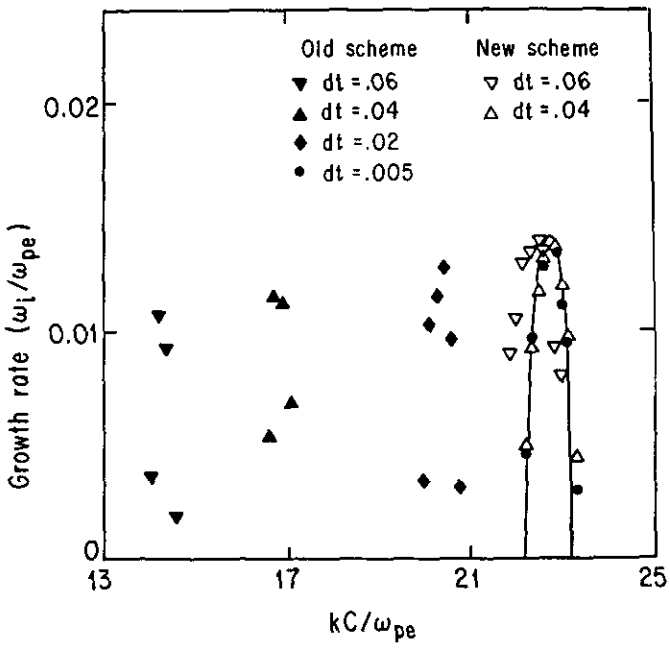

FIG. 6. The growth rates and radiation spectrums observed from the old scheme and the new scheme. The solid line is calculated from the theoretic dispersion relation.

The curve of $\omega_{es} - \omega_{em}$ is nearly a straight line and independent of the size of time step. The frequency error of simulation by the old scheme is approximately increased by the square of the size of time step. The larger is the size of time step; the smaller is the wave number of the intersection point. Figure 6 gives a very consistent result as indicated in Fig. 5. The shift of the radiation spectrum is about 40% compared to the old scheme using $\Delta t = 0.06$ (where we eliminated certain high k modes to make the simulation stable), while $\Delta t = 0.005$ provides a correct radiation spectrum and growth rates. The new scheme generates good spectrum and growth rates by using larger sizes of time step, which are about one order of magnitude larger than that required by the old scheme. A typical run of the 1 2/2 D ion-ripple laser simulation needs $t \sim 4 \times 10^3$ for the waves to saturate. With the old scheme it takes about 30 h Cray time. Now, it costs about 3 h Cray time.

IV. SUMMARY AND DISCUSSION

The new time-differencing with the neo-finite-difference method is applied to a spectral electromagnetic simulation. The new scheme improves both accuracy and stability. In fact, it is theoretically unconditionally stable. The size of the time step is not restricted by the stability condition of standard spectral methods. The limitation on the time step will only depend on the temporal resolution requirement of physical quantities, which do not cause numerical instability.

Before we test the new scheme, the errors of electromagnetic wave frequency induced by the old scheme in particle-in-cell simulations are estimated. The simulation results show that their errors are about the same as the errors predicted by the estimation. A strong numerical instability occurs as the size of time step in the old scheme simulation is too large to satisfy the stability condition of the standard time-differencing method. The numerical shifts of the radiation spectrum in an ion-ripple laser are observed in the old scheme simulation and are due to the frequency errors. As our new scheme corrects the frequency errors, a stable numerical simulation has been achieved and the radiation spectrum is shown to be correct, even when a large time step is used. In our example, the size of time step in the new scheme can be one order of magnitude larger than the one in the old scheme (about 3 h Cray time per typical run instead of 30 h).

This new scheme does not increase computation time per time step because we only need to change two statements concerning the form factor in our existing code.

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