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A Courant Condition-Free Modified Partially Implicit Method. Revised Electromagnetic Particle Code PS2M for Bounded Plasmas with Conducting Walls

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The distortion of the dispersion of the light waves or the nonphysical frequency alias is shown to exist in the Courant condition relaxed methods already proposed. A new method for correcting this distortion without generating the alias is proposed. The proposed method is obtained by merging the merit of one type of method (the spectral method) to another type of method (the difference method). © 1990 Academic Press, Inc.

The distortion of the dispersion of the light waves or the nonphysical frequency alias exists in the Courant condition relaxed methods already proposed [1–6]. In this paper, a method for correcting this distortion without generating the alias is proposed. The proposed method is obtained by merging the merit of one type of method [2–5] to another type of method [1].

In order to devise this method, a set of difference equations with interesting features is first given and is then modified to a finite-difference approximation for the time integration of the Maxwell equations without affecting the numerical stability and without generating the nonphysical frequency alias. The new method includes the merits of both types of methods and excludes their faults which appear in expanding the time step far beyond the Courant condition. As an application, this method is embodied in a code PS2M [7], which is a particle simulation code in 2.5 dimensions (2 space dimensions and 3 velocity dimensions) for electromagnetic plasmas with a pair of parallel conducting plates (a slab model).

Nielson and Lindman [1] have developed the 2-dimensional electromagnetic code, in which the Maxwell equations are differenced implicitly with respect to time only for the transverse quantities [7], while the equations for the longitudinal quantities [7] and the equations of motion for the charged particles are differenced explicitly. (In this paper, we call a method, which adopts such difference equations for the time integration, a partially implicit method for convenience.) This method

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is less subject to the limit of the Courant condition, i.e., $ck_{\max} \Delta t < 2$, where c, $k_{\max}$, and Δt are the light speed, the maximum wave number in the system, and a time step. They also proposed a method to remedy the distortion of the dispersion relation for the high-frequency modes in the partially implicit method in which the field equations are solved by differencing the Maxwell equations for the spatial variables. This method is referred to as the difference method in this paper.

On the other hand, for the spatially periodic system, Lee, Boris, and Haber *et al.* [2], Lin, Okuda, and Dawson [3], Buneman *et al.* [4], and Birdsall and Langdon [5] proposed alternative methods. In common, these methods adopt the computational method in which the field equations are integrated spatially by using the Fourier expansion. In these methods, referred as to the spectral methods, the Maxwell equations can be exactly integrated with respect to time for each Fourier-expanded mode, which has an exact dispersion relation for the light waves in a vacuum, if $ck_{\max} \Delta t < \pi$.

The latter methods (spectral methods) may be more exact for remedy of the distortion of the numerical dispersion relation than the former method (the difference method[1]) and may be preferred, if $ck_{\max} \Delta t < \pi$.

However, as will be shown later, the spectral methods have a defect that the non-physical frequency alias appears for the electromagnetic modes with $ck \Delta t > \pi$, which are often required to be simulated, as an example is introduced in the following: In the simulation of certain phenomena such as the plasma heating or the non-inductive current drive by the electron cyclotron range of frequency waves, the long-wavelength electromagnetic waves and the short-wavelength electrostatic waves coexist in a system. In this case, we easily meet a serious problem how we simulate the system with the parameter $ck_{\max} \Delta t \geqslant \pi$, when we use a large time step of $\omega_{pe} \Delta t \sim 1$ in the case of $ck_{\max} > \pi\omega_{pe}$, i.e., $M^{1/2}c/\Delta > \omega_{pe}$, where Δ is a grid spacing and M is a spatial dimension of the model. Therefore, it is desirable to make a model in which the Courant condition is relaxed without distortion of the wave dispersion and without the frequency alias.

Through our attempt in the previous and present works on PS2M [6–9], we coherently aim at making a comparably versatile model in which the full electron dynamics is retained. In the fully implicit method recently developed extensively, the plasma oscillation and the electron cyclotron motion are filtered out in time. The linear phenomena of the low frequency may be well described by these models, while there may exist the case that these models cannot be applied to wide areas of the nonlinear plasma physics even in the low-frequency phenomena. We have found one typical example which is explained later.

[1] In this difference method, there exist cases that the numerical stability is regressed when the distortion of the numerical dispersion relation is remedied. In other words, it cannot be said that this method is always stable if $\omega_{pe} \Delta t < 2$. Furthermore, Nielson and Lindman's method is effective for the spatially differenced Maxwell equations; however, we know from our own study that it loses effectiveness regarding the remedy of the dispersion when we apply it to the system in which the field equations are integrated spatially by using the Fourier expansion.

Here, we will introduce a new method of the time integration of the Maxwell equations for the electromagnetic code in which the boundary value problems are solved by using the eigenfunction expansions which are expanded by the Fourier modes defined in the full period and the half period. A proper use of expansion by the Fourier modes defined in the half period makes a conducting boundary condition, as described in Ref. [7]. Extending the definition of the wave number $\mathbf{k}$ from the real number to the complex number [7, 9], we get $\mathbf{k}$ concerning the Maxwell equation for the conducting wall boundary,

$$\mathbf{k} = (ik_m, k_n, 0), \tag{1}$$

where

$$k_m = \frac{\pi m}{L_x}, \qquad k_n = \frac{2\pi n}{L_y}. \tag{2}$$

Here it is assumed that the system is bounded by a pair of conducting walls in the x direction, periodic in the y direction, and uniform in the z direction with system size of $L_x \times L_y$.

We modify the implicit difference equations given by Nielson and Lindman [1] in order to remove the Courant restriction of $ck_{\max}\Delta t < 2$ and to remedy the distortion of numerical dispersion relation of the light waves without affecting its numerical stability and without generating frequency alias. Thus, we get new difference equations for the Maxwell equations which are written as

$$\begin{aligned}&\frac{\{\mathbf{E}_k{}^{\mathrm{T}}\}_N - \{\mathbf{E}_k{}^{\mathrm{T}}\}_{N-1}}{\Delta t}\\ &\quad = ic^2 f(k)\mathbf{k} \times [\beta\{\mathbf{B}_k{}^{\mathrm{T}}\}_N + (1-\beta)\{\mathbf{B}_k{}^{\mathrm{T}}\}_{N-1}] - \frac{1}{\varepsilon_0}\{\mathbf{J}_k{}^{\mathrm{T}}\}_{N-1/2},\end{aligned} \tag{3}$$

$$\begin{aligned}&\frac{\{\mathbf{B}_k{}^{\mathrm{T}}\}_N - \{\mathbf{B}_k{}^{\mathrm{T}}\}_{N-1}}{\Delta t}\\ &\quad = -if(k)\mathbf{k}^* \times [\gamma\{\mathbf{E}_k{}^{\mathrm{T}}\}_N + (1-\gamma)\{\mathbf{E}_k{}^{\mathrm{T}}\}_{N-1}],\end{aligned} \tag{4}$$

where $\mathbf{E}_k{}^{\mathrm{T}}$, $\mathbf{B}_k{}^{\mathrm{T}}$, and $\mathbf{J}_k{}^{\mathrm{T}}$ are the coefficients of the Fourier series expansion or the eigenfunction expansion of the electric and magnetic fields and the current density, respectively. The superscript T denotes the transverse component [7] of each vector quantity and the subscript N denotes time $t = N\Delta t$. The numerical stability condition requires $\frac{1}{2} \leqslant \beta$, $\gamma \leqslant 1$. The function $f(k)$ is the correction function. The vector $\mathbf{k}^*$ is the complex conjugate of the wave number vector $\mathbf{k}$. The scalar k is defined as $k = (\mathbf{k} \cdot \mathbf{k}^*)^{1/2}$. (If the system is periodic in both the directions, the whole discussion holds if k_m is set to be $k_m = -2\pi i m/L_x$ in Eq. (2).)

The introduction of $f(k)$ which depends on k is a key point, compared with our previous proposal [6]. The proper choice of functions $f(k)$ can significantly improve the dispersion relation of the simulated plasma without generating the frequency alias.

When the correction function $f(k)$ is chosen as

$$f(k) = \tan \zeta/\zeta \qquad \text{and} \qquad \beta = \gamma = \tfrac{1}{2}, \tag{5}$$

where

$$\zeta = \frac{ck\,\Delta t}{2}, \tag{6}$$

it can be shown that the formulation presented in this paper is identical with the special case of that presented by Birdsall and Langdon, i.e., with the case of $\alpha(k) = \cos(ck\,\Delta t/2)$ in Ref. [5], where $\alpha(k)$ is a spatial filtering function for the current density **J** defined in their expression [5]. Thus, these difference equations have an interesting feature that their solution also satisfies exactly the original Maxwell differential equations at $t = N\,\Delta t$, if $ck\,\Delta t \leqslant \pi$. Birdsall and Langdon [5] point out that, unless $\alpha(k)$ is sufficiently small near multiples of π for $ck\,\Delta t$, the numerical instability appears not in vacuum but in the pla1smas as in the case of $\alpha(k) = \sin(ck\,\Delta t/2)/(ck\,\Delta t/2)$ which corresponds to the schemes proposed in Refs. [2, 4, 5]. However, when $\alpha(k)$ is chosen to be $\alpha(k) = \cos(ck\,\Delta t/2)$, which is written first, Birdsall and Langdon's method is stable for the system with $\omega_{pe}\,\Delta t < 2$. Therefore, the difference equations, Eqs. (3) and (4) with Eq. (5), are also stable not only in vacuum but also in the plasmas. To our regret, however, we have another new problem instead for the solution of the difference equations. Although there exist no descriptions in the book [5], we have found a serious drawback that the frequency alias appears surely for the electromagnetic modes with $ck\,\Delta t > \pi$. This frequency alias originates from the property of the function $\tan \zeta$, which has a periodicity with respect to its argument $\zeta = ck\,\Delta t/2$.

The high-frequency alias with frequency of $\omega\,\Delta t > 2$ is not so serious, because it may be considered to be a kind of noise, while the low-frequency alias appearing around $ck\,\Delta t = 2n\pi$ (n is an integer) may distort the original plasma physics, as is shown later. This is a reason why we consider that the previous spectral methods [2–5] have a fault when we expand the time step sufficiently, compared with the conventional difference scheme with the Courant limit.

Because a mild remedy of the wave dispersion can avoid the generation of frequency alias, we adopt the following function of the finite series of ζ as $f(k)$ whose number of the maximum order on ζ is N_ζ,

$$f(k) = 1 + \frac{1}{3}\zeta^2 + \frac{2}{15}\zeta^4 + \frac{17}{315}\zeta^6 + \cdots + \frac{(-1)^{n-1}2^{2n}(2^{2n}-1)\,B_{2n}}{(2n)!}\zeta^{2(n-1)}, \tag{7}$$

where B_n is the Bernoulli number and $n = N_\zeta$.

The function $f(k)$ defined by Eq. (7) is obtained by expanding $\tan \zeta/\zeta$ to an infinite series and truncating it with the finite order N_ζ. As N_ζ increases, the distortion of the dispersion relation decreases, as is easily understood.

When the correction function $f(k)$ is the lowest order with respect to ζ, i.e., $N_\zeta = 0$ as

$$f(k) = 1 \qquad \text{and} \qquad \beta = \gamma = \tfrac{1}{2}, \tag{8}$$

the formulation of the field equations is reduced to the special case of the formulation presented by Nielson and Lindman ($\alpha^2 = 0$ in Ref. [1]) and was studied in Ref. [6].

Although the function $f(k)$ defined by Eq. (7) is derived by Taylor-expanding $\tan\zeta/\zeta$, it differs remarkably from $f(k) = \tan\zeta/\zeta$ for $\zeta > \pi/2$ $(k > \pi/c\,\Delta t)$; in other words, $f(k)$ defined by Eq. (7) increases monotonically with ζ for $k > \pi/c\,\Delta t$. This property of the function $f(k)$ defined by Eq. (7) eliminates the frequency aliasing observed in the method presented by Birdsall and Langdon [5] in the case of $k_{\max} > \pi/c\,\Delta t$, as will be shown later.

The current density $\mathbf{J}_{N-1/2}$ is calculated from the velocity and the position of the jth particle, $\mathbf{v}_{j\sigma,N-1/2}$ and $\mathbf{r}_{j\sigma,N-1/2} = (\mathbf{r}_{j\sigma,N-1} + \mathbf{r}_{j\sigma,N})/2 = \mathbf{r}_{j\sigma,N-1} + \Delta t/2\mathbf{v}_{j\sigma,N-1/2}$ as

$$\mathbf{J}_{N-1/2} = \sum_\sigma q_\sigma \sum_j \mathbf{v}_{j\sigma,N-1/2} W_g(\mathbf{r}, \mathbf{r}_{j\sigma,N-1/2}). \tag{9}$$

Here, $W_g(r, r_j)$ is the weighting function of the particle in a gridded system [8].

The longitudinal component $\mathbf{E}^L_N$ [7] is calculated as

$$\nabla \cdot \mathbf{E}^L_N = \frac{\rho_N}{\varepsilon_0}, \tag{10}$$

where

$$\rho_N = \sum_\sigma q_\sigma \sum_j W_g(\mathbf{r}, \mathbf{r}_{j\sigma,N}). \tag{11}$$

The particle velocity $\mathbf{v}_{j\sigma,N+1/2}$ and its position $\mathbf{r}_{j\sigma,N+1}$ are obtained by using the methods proposed by Buneman [10] and Boris [11].

Figure 1 shows an example of the numerical dispersion relation in which the modified partially implicit formulation is used as for the Maxwell equation. The plasma is assumed to be a magnetized cold electron plasma. The derivation of this numerical dispersion relation and its detailed property will be given elsewhere [9]. In Fig. 1, the numerical solution of this dispersion relation is presented for various N_ζ. The ions are assumed to be an immobile background. The parameters are $\beta = \gamma = \frac{1}{2}$, $\Delta = 1.0$, $c\,\Delta t/\Delta = 6$ $(ck_{\max}\,\Delta t = 6\pi)$, $\omega_{pe}\,\Delta t = 0.405$, $\Omega_e/\omega_{pe} = 1.5$. $k_{\parallel} = 0$, where ω_{pe} and Ω_e are the electron plasma and cyclotron frequencies, respectively. Solid lines show a dispersion relation calculated in the case of the infinitesimal time step $\Delta t = 0$. From the top, the solid lines indicate two light waves (fast extraordinary and ordinary modes) and a slow extraordinary mode.

When $\omega\,\Delta t$ is larger than unity, the distortion of the light waves due to the finite-time-step effects is obvious for $N_\zeta = 0$. However, as N_ζ increases, the distortion of the dispersion relation of the light waves decreases.

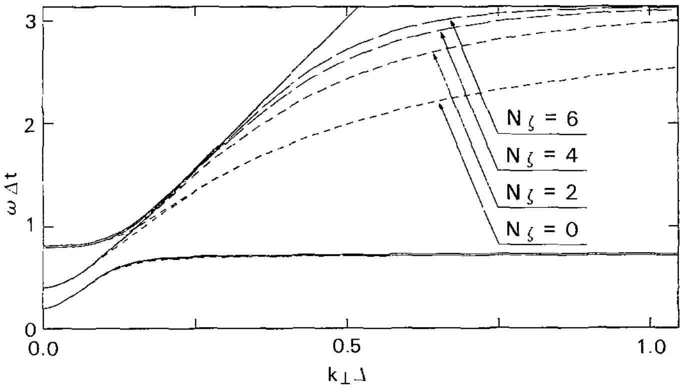

FIG. 1. The dashed lines show the numerical dispersion curves of the waves traveling perpendicular to the magnetic field for the partially implicit ($N_\zeta = 0$) and for the modified partially implicit ($N_\zeta = 2, 4, 6$) formulations. The solid lines indicate the dispersion curves in the case of $\Delta t = 0$.

In order to illustrate the remedy of the distortion of the dispersion relation of the light waves, we will present the simulation results for propagation of the electromagnetic waves and compare them with the theoretical calculation. The simulation results, which are obtained by using Birdsall and Langdon's method [5], are also presented to show that the aliasing phenomena can be actually observed and are significant.

In order to excite the electromagnetic waves which are the ordinary waves and the fast and slow extraordinary waves traveling perpendicularly to the magnetic field $\mathbf{B}_0 = B_0\hat{y}$, the external source current is located inside the plasma at $x_0 = 250\Delta$. The frequencies of the external current density are multiple, i.e., the external current is represented by the superposition of each sinusoidal component

$$\mathbf{J}_{ext}(x, y, t) = J_0(\hat{y} + \hat{z})\,\delta(x - x_0)\sin(\omega_0 t). \tag{12}$$

The frequencies of the external current are $\omega_0 \Delta t = 0.48$, 0.72, 1.05, 1.35, and 1.65. An absorbing boundary condition [12] is imposed on the electromagnetic field at the left and right boundaries ($0 \leqslant x/\Delta \leqslant 240$, $784 \leqslant x/\Delta \leqslant 1024$) in order to prevent reflection of the electromagnetic waves at the conducting walls.

Figure 2 shows the interferograms between the external source current component with frequency of $\omega_0 \Delta t = 1.65$ and the transverse field E_z^T [7], which corresponds to the fast extraordinary wave. The absorbing boundary condition forces the waves to damp in the region of $0 \leqslant x/\Delta \leqslant 240$ and $780 \leqslant x/\Delta \leqslant 1024$, before the waves reach the conducting boundaries. As shown in Fig. 2a, the aliasing effect are obvious for the Birdsall and Langdon's method [5]; the wave with the short wavelength ($\lambda_\perp/\Delta = 8.00$) is superposed on the waves with the long wavelength ($\lambda_\perp/\Delta = 23.3$), while the wavelength of the fast extraordinary wave numerically calculated is $\lambda_\perp/\Delta = 23.7$. This is an example that the original plasma physics is distorted due to appearance of the mode which should not exist in the natural plasma.

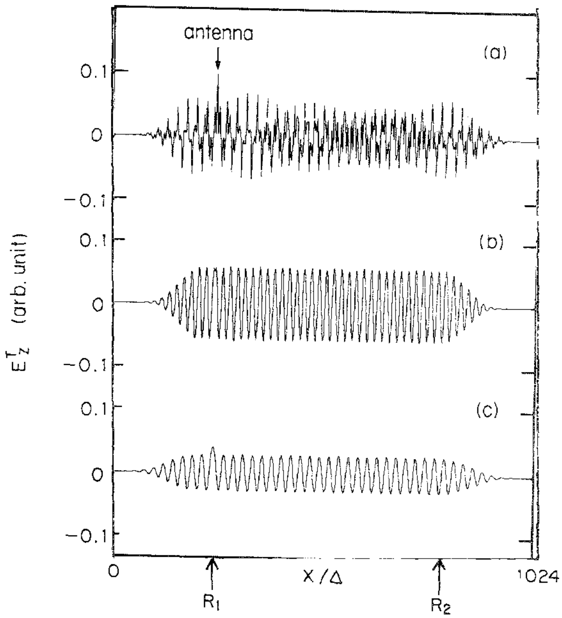

FIG. 2. Interferograms of the transverse (electromagnetic) field E_z^T at $t = 137\ (2\pi/\omega)$. The simulation results obtained by using the following three methods: (a) Birdsall and Langdons' method; (b) the partially implicit method ($N_\zeta = 0$); (c) the modified partially-implicit method ($N_\zeta = 6$).

For the partially implicit method ($N_\zeta = 0$) and the modified partially implicit method ($N_\zeta = 6$), on the other hand, the aliasing effects are not observed, as shown in Figs. 2b and c.

In Fig. 3, the wave numbers $k_\perp$, measured in the region of $300 \leqslant x/\Delta \leqslant 556$ by the use of a relation of $k_\perp = \lambda_\perp/2\pi$, are shown by the circles and triangles, which are measured from the interferograms of E_z^T and E_y^T, respectively. The solid and the dashed curves indicate the numerical solution of the dispersion relations without the finite-time-step effects and with the finite-time-step effects, respectively.

As seen in Fig. 3a for the Birdsall and Langdon's method [5], the aliasing effect, which is predicted from the numerical solution of dispersion relation, produces a pair of modes with the same wave frequency in this system. The mode with lower k is usual normal mode and the mode with higher k is an aliasing mode. As seen in Figs. 3b and c for the partially implicit and the modified partially implicit methods ($N_\zeta = 0$ and $N_\zeta = 6$), the elimination of the aliasing effects is shown in the simulation results as expected from the numerical solution of the dispersion relation. The distortion of dispersion relation of the light waves is confirmed for the partially implicit method ($N_\zeta = 0$), as shown in Fig. 3b, and the remedy of this distortion in the region of $\omega\,\Delta t \leqslant 2$ is confirmed for the modified partially implicit method ($N_\zeta = 6$), as shown in Fig. 3c.

In the usual plasma parameters, we do not need to use the retarded time difference of $0.5 < \beta$, $\gamma \leqslant 1.0$. However, when we want to simulate plasmas with the

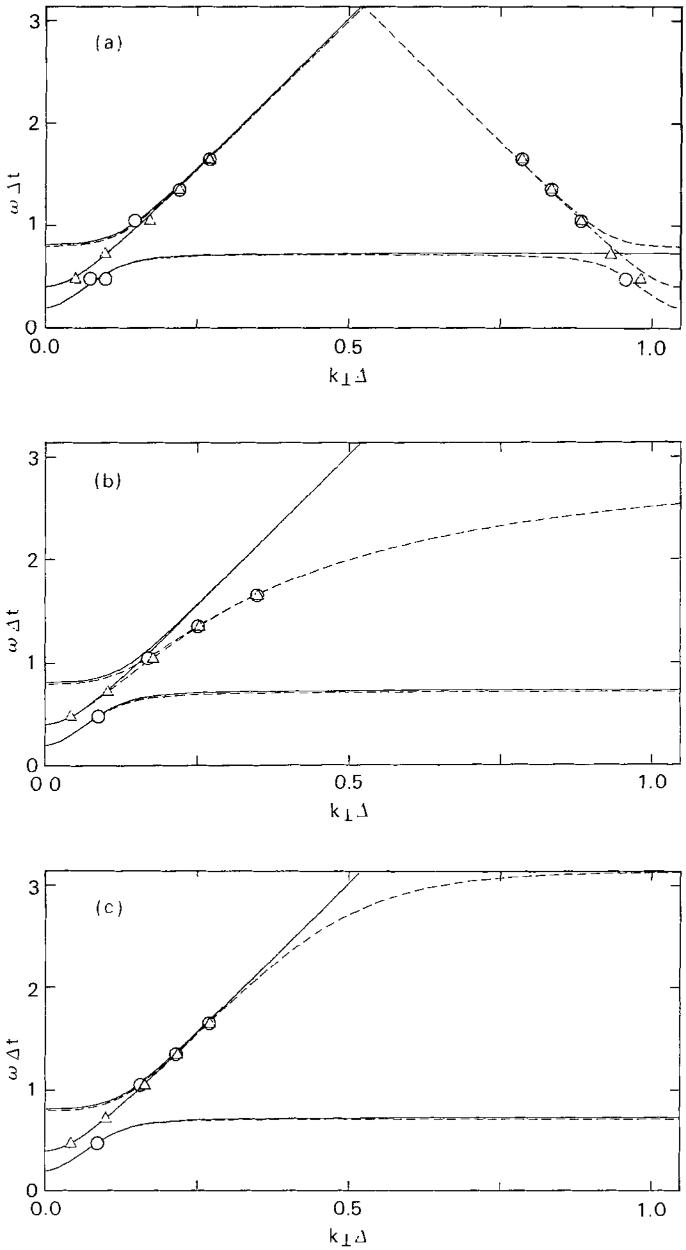

FIG. 3. Comparison between the numerical dispersion curve and the simulation results. The solid and the dashed curves indicate the numerical solution of the dispersion relations without the finite-time-step effects and with the finite-time-step effects, respectively. The circles and the triangles indicate the simulation results at $t = 137\ (2\pi/\omega)$ and correspond to $k_\perp$ measured from the interferograms of $E_z^{\rm T}$ and $E_y^{\rm T}$, respectively: (a) Birdsall and Langdons' method; (b) the partially implicit method ($N_\zeta = 0$); (c) the modified partially implicit method ($N_\zeta = 6$).

relativistic, extremely high electron temperature or high energy electron beam, we should consider the occurrence of the numerical Cherenkov instabilities, which are studied by Godfrey [13]. In this case, the retarded time difference scheme of $0.5 < \beta$, $\gamma \leqslant 1.0$ may be effective in order to suppress this numerical instability, although this method has not been tested yet.

Note that the method proposed here cannot be substituted by, for example, the combination of the Birdsall and Langdon's method and the high-k cutoff method for the modes with $ck\,\Delta t > \pi$, because the high-k cutoff method eliminates not only the unnecessary high-frequency and high-k modes but also the necessary low-frequency and high-k modes, one example of which is the slow extraordinary mode (see Fig. 1).

The proposed difference equations, Eqs. (3) and (4), for the Maxwell equation are very conveneient and useful, because its form is tractable and is easy to understand its physical meaning. When we difference the Maxwell equation spatially, we get a better formulation by replacing $-k^2$ with ∇^2 in Eq. (7), although we have not yet pursued this idea in detail. These difference equations may be applied to other models such at the fully implicit electromagnetic model.

We remark the property of the PS2M code [7] revised by using the method proposed here. When $\beta = \gamma = \frac{1}{2}$, the high-frequency electromagnetic modes are not filtered out in time, but their phase velocities are less than the light speed c and their group velocities approach zero in high-k modes as a result of modification of their dispersion relation due to the use of the stabilized difference equations. The noise level associated with this high-frequency transverse electric field [7] is less than that with the longitudinal electric field [7] and is small enough to little alter the collective phenomena which are desired to simulate [9].

The plasma oscillation is retained in the system unlike the fully implicit method in which the plasma oscillation is filtered out in time. The scheme for the whole time stepping is still time-centered in the case of $\beta = \gamma = \frac{1}{2}$ which is usually used, although a part of the field equations are implicitly integrated in time. The restriction for the spatial grid length is relaxed by using the high-order spline [8]. Thus, Ref. [9] has shown that the remaining restriction on the simulation parameter both for the magnetized and for the unmagnetized cold plasmas is $\omega_{pe}\,\Delta t \leqslant 2.0$, although a practical and safe time step may be decreased to $\omega_{pe}\,\Delta t \leqslant 1.0$ due to the thermal effects and so on. We have many problems in the laboratory plasmas and the space plasmas in which the condition of $\omega_{pe}\,\Delta t \leqslant 1.0$ is a physical requirement. As examples, this code, PS2M, has been used to study RF stabilization of flute modes [14, 15] and ECRH [16, 17, 18], where the partially implicit method of $N_\zeta = 0$ is used for part of runs with time steps which are so moderate that the wave dispersions are not affected. The reliability and the usefulness of the method proposed are verified in the success of expanding the time step. Especially, Ref. [15] is the typical example that the full electron dynamics is very important even for the ion cyclotron range frequency phenomenon because the full perpendicular electron dynamics cannot be substituted by the temporally averaged motion without the RF electric fields for the nonlinear phenomena such as the RF stabilization and destabilization of the flute mode due to the ponderomotive force and sideband coupling effects. Recently, the modified partially implicit method of order 6 ($N_\zeta = 6$) is also used for the non-inductive current drive by ECRH [20, 21]. In this case, a simulation parameter with the time step large enough to detect difference between the dispersions of the pumping wave for two methods is tested. The two results are compared and a significant difference is observed for current generation efficiency. Therefore, we should properly use both the methods of $N_\zeta = 0$ and $N_\zeta = 6$ according to each purpose. The partially implicit method of $N_\zeta = 0$ is still useful enough to simulate the low-frequency phenomena when the moderate time step is used.

The specialization of this method to the 1-dimensional case is trivial and has been already implemented as an option of PS2M. The generalization to the 3-dimensional case is clearly straightforward and will be implemented in the future.

Here we summarize this paper. First, we have pointed out a problem on existence of the nonphysical frequency alias for the spectral method already proposed [2–5]. This problem has been neglected for about 15 years, although it is very serious. Second, we have given a set of difference equations, Eqs. (3) and (4) with Eq. (5) in order to devise a new method. Third, we have proposed a method in which Eq. (7) is adopted instead of Eq. (5) and embodied it in the particle code PS2M [7] and verified that the proposed method is improved, compared with the previous [1–6], for correcting distortion of the dispersion of the light waves without generation of the nonphysical frequency alias.

Finally, we comment on the proper use for our new method and the previously proposed method. Our algorithm is important only because it is pushing the time step limit beyond $ck_{\max} \Delta t > \pi$. This is a relatively unexplored and new regime. For the codes in the regime of $ck_{\max} \Delta t < \pi$, Birdsall and Langdon's scheme [5] is still preferable.

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