ON THE IMPORTANCE OF FOURTH ORDER EFFECTS ON WAKEFIELD CALCULATIONS FOR SHORT BUNCHES*

Zenghai Li and Joseph J. Bisognano
CEBAF, 12000 Jefferson Avenue, Newport News, VA 23606

Abstract

The second-order FD-TD algorithm developed by Yee has been successful in wakefield calculations. However, unphysical results can be obtained in wakefunction calculations of very short bunches. A detailed study of this problem is presented in this paper. It is found that the truncation error inherent in the second-order Yee algorithm of standard codes is frequency dependent and is inadequate for wakefield calculations of short bunches which produce wakefields with high frequencies. A fourth order approach extending the work of J. Fang is presented, which reduces the truncation error two orders of magnitude. The results of the wakefunctions calculated by use of this fourth-order FD-TD algorithm are presented and compared with the results of the second-order FD-TD algorithm.

I. INTRODUCTION

Wakefunctions describe energy loss and transverse momentum change which a particle experiences when passing through a structure. Numerical calculations typically use a linear finite-difference time-domain (FD-TD) algorithm, known as the Yee [1] algorithm, to solve the Maxwell's equations. The algorithm has second order accuracy and has been widely used in numerical modeling of electromagnetic wave (microwave) interactions with arbitrary structures and beam-cavity interactions. The algorithm usually gives very good results by choosing an appropriate mesh and time step size. In the application of modeling microwave structures, good accuracy can be obtained by having the mesh size one tenth of λ_{min} [2]. In the application of wakefields calculations, good accuracy can be obtained by having the mesh size one fifth of σ, where σ is the rms bunch length of the driving particles, assuming a gaussian distribution.

Problems arise when the fields have high frequency components. These were encountered in the wakefields evaluations of the CEBAF 5-cell cavities. The CEBAF beam has very short bunch length. The spectrum of the current carried by the bunch contains very high frequency components. The wakefunctions calculated by use of TBCI and ABCI have unphysical oscillations even if the mesh size is one fifth of the rms bunch length.

It is found that these unphysical oscillations are due to the accuracy of the Yee algorithm and are frequency dependent. To solve the problem, we, extending J. Fang's work [3], developed a fourth-order finite-difference formalism in the cylindrical coordinate system. This formulae have accuracy to the forth order.

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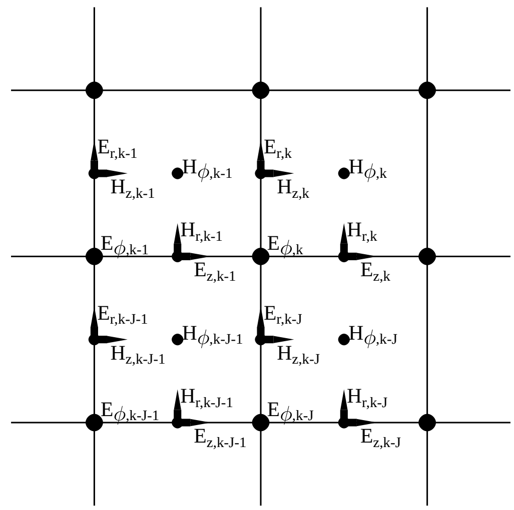

Figure. 1. The fields defined in the $r - z$ plane.

II. THE SECOND-ORDER FD-TD ALGORITHM

In this section, we present the FD-TD formulae in the cylindrical coordinate system used in TBCI [4]. The second-order FD-TD algorithm approximates the first-order time and spatial derivatives by linear finite differences. On the time axis, the H fields are evaluated a half time step ahead of the E fields, which gives a centered-difference analog to the time derivatives. Let the H fields be evaluated at times $n\Delta t$ and the E fields at times $(n + 1/2)\Delta t$, n =1, 2, 3.... The Maxwell's equations become

$$\mathsf{H}^{n+1} = \mathsf{H}^{n} - \frac{\Delta t}{\mu_0}\nabla \times \mathsf{E}^{n+1/2} \quad (1)$$

$$\mathsf{E}^{n+3/2} = \mathsf{E}^{n+1/2} + \frac{\Delta t}{\epsilon_0}\nabla \times \mathsf{H}^{n+1} - \frac{\Delta t}{\epsilon_0}\mathsf{J}^{n+1} \quad (2)$$

The fields are treated analytically in the ϕ coordinate, and are discretized in the $r - z$ plane as shown in Fig. 1. The first order derivatives in the curl operators in Eqs. (1) and (2) are replaced by linear finite differences

$$\frac{\partial(E, H)}{\partial x_i} \rightarrow \frac{(E, H)_{j+1} - (E, H)_j}{\Delta x_i} \quad (3)$$

The arrangement of the E and H fields in Fig. 1 provides a natural geometry which fulfills the centered-difference analog to the spatial derivatives of the curl operators in Maxwell's equations. The centered-difference scheme has accuracy to the second order.

To calculate the wakefield of a particle bunch, the fields are initially set to zero, $\mathsf{E}^{1/2} = 0$, $\mathsf{H}^{0} = 0$, $\mathsf{J}^{0} = 0$. The total electromagnetic fields can be calculated iteratively over these difference equations through the leapfrog process set forth by the centered-difference in the time axis.

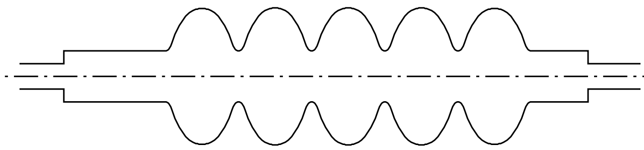

Figure. 2. The cross section of the CEBAF 5-cell cavity.

The wakefunctions of the CEBAF superconducting cavity are calculated to demonstrate the shortcomings of the second-order FD-TD algorithm. The cross section of the CEBAF 5-cell cavity is as shown in Fig. 2. The mesh size used in the calculations is one fifth of the rms bunch length. The beam is on the axis. The wake is integrated at the beam pipe radius. The dashed line in Fig. 3 shows the longitudinal wakefunction of mode $m = 0$ for a 0.5 mm (rms) beam. The dotted line is the charge distribution. The wakefunction has strong oscillations starting from the tail of the bunch. These oscillations are unphysical since the strength is stronger than the wakefunction in the bunch region. The wakefunction calculated by TBCI for a 3 mm (rms) beam does not have the same problem, Fig. 4. This suggests that the error is bunch length dependent.

III. FOURTH-ORDER FD-TD ALGORITHM

Further studies showed [5] that the unphysical oscillations of the wakefunction in Fig. 3 is due to the truncation error of the second-order FD-TD algorithm. In principle, the problem can be solved by using a finer mesh. This may be impractical due to the limitation of computer memory. In this section, we derive a fourth-order FD-TD algorithm in the cylindrically symmetric coordinate system. The Yee lattice is used to define the fields. Fourth order accuracy is accomplished by including up to the third order derivatives of the fields in the Taylor expansions.

A. Fourth-order FD-TD algorithm

Expanding the E and the H fields to third order in time, we have

$$\mathsf{H}^{n+1} = \mathsf{H}^{n} + \Delta t \frac{\partial \mathsf{H}^{n+1/2}}{\partial t} + \frac{\Delta t^3}{24}\frac{\partial^3 \mathsf{H}^{n+1/2}}{\partial t^3} + O(\Delta t^5) \quad (4)$$

$$\mathsf{E}^{n+3/2} = \mathsf{E}^{n+1/2} + \Delta t \frac{\partial \mathsf{E}^{n+1}}{\partial t} + \frac{\Delta t^3}{24}\frac{\partial^3 \mathsf{E}^{n+1}}{\partial t^3} + O(\Delta t^5) \quad (5)$$

Replacing the time derivatives in Eqs. (4,5) by the curl operators defined by the Maxwell's equations, we have

$$\mathsf{H}^{n+1} = \mathsf{H}^{n} - \frac{\Delta t}{\mu_0}\nabla \times \mathsf{E}^{n+1/2} - \frac{\Delta t^3 c^2}{24\mu_0}\nabla \times \nabla^2 \mathsf{E}^{n+1/2} + \frac{\Delta t^3 c^2}{24}\frac{\partial}{\partial t}(\nabla \times \mathsf{J}^{n+1/2}) + O(\Delta t^5) \quad (6)$$

$$\mathsf{E}^{n+3/2} = \mathsf{E}^{n+1/2} + \frac{\Delta t}{\epsilon_0}\nabla \times \mathsf{H}^{n+1} + \frac{\Delta t^3 c^2}{24\epsilon_0}\nabla \times \nabla^2 \mathsf{H}^{n+1} - \frac{\Delta t}{\epsilon_0}\mathsf{J}^{n+1} + \frac{\Delta t^3}{24\epsilon_0}\left(c^2 \nabla \times \nabla \times \mathsf{J}^{n+1} - \frac{\partial^2 \mathsf{J}^{n+1}}{\partial t^2}\right) + O(\Delta t^5) \quad (7)$$

The first order derivatives involved in the curl operators are evaluated to the fourth order finite-difference as

$$\frac{\partial H_{z,k+1/2}}{\partial z} = \frac{H_{z,k+1} - H_{z,k}}{\Delta z} - \frac{\Delta z^2}{24}\frac{\partial^3 H_{z,k+1/2}}{\partial z^3} + O(\Delta z^4) \quad (8)$$

B. Frequency dependence of the higher-order terms

For a given mode, assuming that the fields have $e^{-j\omega t}$ time dependence, the third order terms in Eq. (6) have the following form (similarly for the E field in Eq. (7))

$$\begin{aligned}\Delta\left(\frac{\Delta \mathsf{H}}{\Delta t}\right) &= -j\frac{\Delta t^2 \omega^3}{24}\mathsf{H} - \frac{\Delta z^2}{24\mu_0}\Bigg(\frac{\partial^3 E_\phi}{\partial z^3}\mathsf{r}_0 \\ &\quad -\Big(\frac{\partial^3 E_r}{\partial z^3} - (k_r^2 + \frac{2}{r^2})\frac{\partial E_z}{\partial r} + \frac{k_r^2}{r}E_z\Big)\phi_0 \\ &\quad -\Big((rk_r^2 - \frac{1}{r})\frac{\partial E_\phi}{\partial r} + 2k_r^2 E_\phi\Big)\mathsf{z}_0\Bigg) \end{aligned} \quad (9)$$

Except for the phase difference, the third order derivatives respect to z can be written as $k_z^3(E, H)$ and the first order derivative respect to r is approximately $k_r(E, H)$. These higher-order terms are, therefor, proportional to $\omega(k\Delta z)^2$, or, $\omega(\frac{\Delta z}{\lambda})^2$. In general, $(\Delta z/\lambda)^2$ is small and is usually used as a measure of the magnitude of the contributions from the terms related. The situation here now is different, the coefficients of $(\Delta z/\lambda)^2$ linearly increase with the frequency. At high frequencies, these terms may not be "small" any more. Furthermore, the accumulated effects of these terms scale as $L_{cavity}\omega(k\Delta z)^2$ in the wakefunction calculation. The higher-order terms thus become more important in the wakefunction calculation of long structures.

In the second-order Yee algorithm, these terms are the lowest order truncation errors and are frequency dependent. Consider the case of wakefields driven by a gaussian bunch; the profile of the frequency spectrum of such a bunch is also gaussian. Frequencies that have lower magnitudes in the spectrum excite wakefields with lower amplitudes. The wakefields excited by the frequencies higher than a certain frequency will be negligibly small. Assuming this rolloff frequency is the frequency with a magnitude of 1% in the spectrum. The corresponding wave length of this frequency is $\lambda = 2\sigma$. Let the mesh size be one fifth of σ, that is $\Delta z/\lambda = 0.1$. This is the typical number suggested in [2] for numerical simulations of microwave propagation and in [4] for wakefield calculations. This number has been accepted as a general rule in the discretization of Maxwell's equations so that the meshes would have enough frequency resolution. This works fine in the calculation of the wakefields of long bunches where the rolloff frequency of the excitation of the wakefields is low. Good accuracy can be obtained with the choice of $\Delta z = \sigma/5$. In the calculation of wakefields of short bunches, the fields contain higher frequency components. The quantity $T\omega(\frac{\Delta z}{\lambda})^2$, where T is the total integration time, may no longer be small even if $\Delta z = \sigma/5$ or $\Delta z/\lambda = 0.1$ is retained since it depends linearly on the frequency and the integration time. The rule of $\Delta z = \sigma/5$ is no longer valid. This is what we have seen in the examples studied in section II. Using smaller mesh size can improve the accuracy. But reducing the mesh size will increase the number of mesh points by many fold, for example 4 fold in the 2-D problem and 8 fold in the 3-D problems if the mesh size is halved. Computer memory becomes a problem.

The fourth-order FD-TD algorithm can reduce the truncation error to the fourth order

$$\omega \left(\frac{\Delta z}{\lambda} \right)^4 \tag{10}$$

Even though it is also linearly proportional to the frequency, the extra powers of $\Delta z/\lambda$ would greatly reduce the magnitude of the error. If the highest frequency of the excitation is not very high, the terms of the fourth order and higher of $\Delta z/\lambda$ are small.

C. *Wakefunctionss calculated by fourth-order FD-TD algorithm*

The fourth-order FD-TD algorithm was implemented in TBCI for testing. The results of the wakefunctions of the CEBAF 5-cell cavity of a 0.5 mm bunch are shown in Fig. 3 by the solid lines. The dashed lines are the results of the second-order FD-TD algorithm. The same mesh size is used, which is $\sigma/\Delta z$=5. No oscillations are observed in the fourth order result. The errors are suppressed.

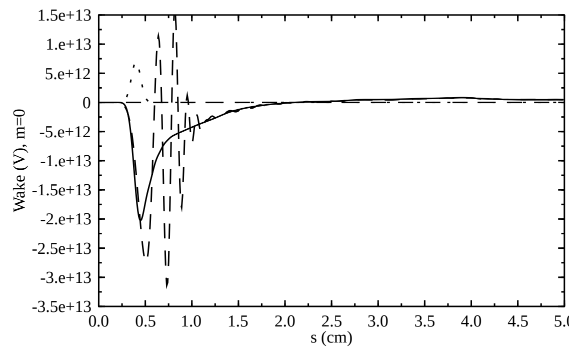

Figure. 3. Wakefunction of the CEBAF 5-cell cavity, σ = 0.5 mm. Dashed line: the result of the second-order FD-TD algorithm; Solid line: the result of the fourth-order FD-TD algorithm.

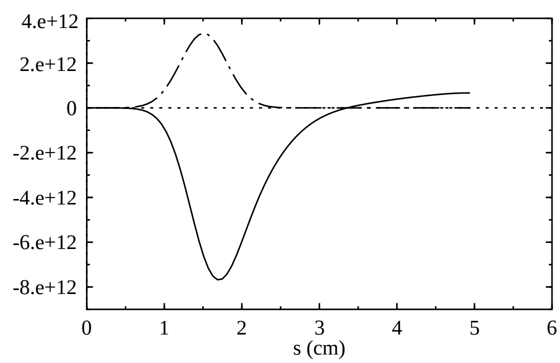

Figure. 4. Wakefunction of the CEBAF 5-cell cavity, σ_z = 3 mm, second-order FD-TD algorithm.

IV. CONCLUSION

Higher-order truncation errors depend linearly on the frequency, and accumulate with time. The fourth-order FD-TD algorithm reduces these errors and is good for calculating the wakefields of sub-millimeter bunches. The fourth-order FD-TD algorithm takes more than six times longer CPU time than the second-order Yee algorithm. In exchange, there is no extra computer memory required.

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