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TE/TM alternating direction scheme for wake field calculation in 3D

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Abstract

In the future, accelerators with very short bunches will be used. It demands developing new numerical approaches for long-time calculation of electromagnetic fields in the vicinity of relativistic bunches. The conventional FDTD scheme, used in MAFIA, ABCI and other wake and PIC codes, suffers from numerical grid dispersion and staircase approximation problem. As an effective cure of the dispersion problem, a numerical scheme without dispersion in longitudinal direction can be used as it was shown by Novokhatski et al. [Transition dynamics of the wake fields of ultrashort bunches, TESLA Report 2000-03, DESY, 2000] and Zagorodnov et al. [J. Comput. Phys. 191 (2003) 525]. In this paper, a new economical conservative scheme for short-range wake field calculation in 3D is presented. As numerical examples show, the new scheme is much more accurate on long-time scale than the conventional FDTD approach.

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1. Introduction

Computation of wake fields of short relativistic bunches in long structures remains a challenging problem even with the fastest computers available. It demands developing new numerical approaches for long-time calculation of electromagnetic fields. The conventional FDTD scheme [3], used in MAFIA [4] and other wake and Particle-In-Cell (PIC) codes, suffers from numerical grid dispersion and the staircase approximation problem. As an effective cure of the dispersion problem, a numerical scheme without dispersion in the longitudinal direction can be used as it was shown in Refs. [1,2].

In this paper, a new two-level economical conservative scheme for short-range wake field calculation in three dimensions is presented. The scheme does not have dispersion in the longitudinal direction and is staircase free (second-order convergent). Unlike the FDTD method [3] and the scheme developed in Ref. [2], it is based on a transversal electric–transversal magnetic (TE/TM)-like splitting of the field components in time. Additionally, it uses an enhanced alternating direction splitting of the transverse space operator that makes the scheme as computationally effective as the conventional FDTD method. Unlike the FDTD ADI method, the splitting error in our scheme is only of the fourth order. As numerical examples show, the new scheme is much more accurate on the long-time scale than the conventional FDTD approach. For axially symmetric geometries, the new scheme performs at least two times faster than the scheme suggested in Ref. [2] achieving the same level of accuracy.

2. Formulation of the problem

At high energies, the particle beam is rigid. To obtain the wake field, the Maxwell equations can be solved with a rigid particle distribution. The influence of the wake field on the particle distribution is neglected here; thus, the beam-surroundings system is not solved self-consistently and a mixed Cauchy problem should be considered.

The problem reads: for a bunch moving with the velocity of light c and characterized by a charge distribution ρ, find the electromagnetic field $\vec{E}, \vec{H}$ in a domain Ω which is bounded transversally by a perfect conductor $\partial\Omega$. The

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bunch introduces an electric current $\vec{j} = \vec{c}\rho$ and thus we have to solve

$$\nabla \times \vec{H} = \frac{\partial}{\partial t}\vec{D} + \vec{j}, \quad \nabla \times \vec{E} = -\frac{\partial}{\partial t}\vec{B}, \quad \nabla \cdot \vec{D} = \rho,$$
$$\nabla \cdot \vec{B} = 0, \tag{1}$$

$$\vec{H} = \mu^{-1}\vec{B}, \quad \vec{D} = \varepsilon\vec{E}, \quad \vec{E}(t=0) = \vec{E}_0,$$
$$\vec{H}(t=0) = \vec{H}_0, \quad x \in \Omega,$$
$$\vec{n} \times \vec{E} = 0, \quad x \in \partial\Omega.$$

3. Implicit numerical scheme

Following the matrix notation of the finite integration technique (FIT) [5], the Cauchy problem (1) can be approximated by the *time-continuous* matrix equations:

$$\mathbf{C}\widehat{\mathbf{e}} = -\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\widehat{\mathbf{b}}}, \quad \mathbf{C}^*\widehat{\mathbf{h}} = \frac{\mathrm{d}}{\mathrm{d}t}\widehat{\widehat{\mathbf{d}}} + \widehat{\widehat{\mathbf{j}}}, \quad \mathbf{S}\widehat{\widehat{\mathbf{b}}} = \mathbf{0},$$
$$\mathbf{S}^*\widehat{\widehat{\mathbf{d}}} = \mathbf{q}, \quad \widehat{\mathbf{e}} = \mathbf{M}_{\varepsilon^{-1}}\widehat{\widehat{\mathbf{d}}}, \quad \widehat{\mathbf{h}} = \mathbf{M}_{\mu^{-1}}\widehat{\widehat{\mathbf{b}}}. \tag{2}$$

With changing of variables, system (2) reduces to the skew-symmetric one:

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{e} = \mathbf{C}_0^*\mathbf{h} + \mathbf{j}, \quad \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{h} = -\mathbf{C}_0\mathbf{e}, \quad \mathbf{e} = \mathbf{M}_{\varepsilon^{-1}}^{-1/2}\widehat{\mathbf{e}},$$
$$\mathbf{h} = \mathbf{M}_{\mu^{-1}}^{-1/2}\widehat{\mathbf{h}}, \quad \mathbf{j} = \mathbf{M}_{\varepsilon^{-1}}^{1/2}\widehat{\widehat{\mathbf{j}}}, \quad \tau = ct. \tag{3}$$

System (3) is a *time-continuous* and *space-discrete* approximation of problem (1). The next step is a discretization of the system in time. The field components can be split in time and the "leap-frog" scheme can be applied. Below two kinds of the splitting are considered: electric–magnetic (E/M) and TE/TM schemes.

As suggested by Yee [3], the E/M splitting of the field components yields the *explicit* FDTD scheme (E/M scheme):

$$\mathbf{e}^{n+0.5} = \mathbf{e}^{n-0.5} + \Delta\tau\,\mathbf{C}_0^*\mathbf{h}^n + \Delta\tau\,\mathbf{j}^n,$$
$$\mathbf{h}^{n+1} = \mathbf{h}^n - \Delta\tau\,\mathbf{C}_0\mathbf{e}^{n+0.5}. \tag{4}$$

Scheme (4) is a two-layer scheme:

$$\mathbf{B}\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta\tau} + \mathbf{A}\mathbf{y}^n = \mathbf{f}^n, \quad \mathbf{B} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \Delta\tau\,\mathbf{C}_0 & \mathbf{I} \end{pmatrix},$$
$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & -\mathbf{C}_0^* \\ \mathbf{C}_0 & \mathbf{0} \end{pmatrix}, \quad \mathbf{y}^n = \begin{pmatrix} \mathbf{e}^{n-0.5} \\ \mathbf{h}^n \end{pmatrix}, \quad \mathbf{f}^n = \begin{pmatrix} \mathbf{j}^n \\ \mathbf{0} \end{pmatrix}.$$

Discrete energy of electromagnetic fields can be defined as

$$E_{\mathrm{E/M}}^n = 0.5\langle[\mathbf{B} - 0.5\Delta\tau\,\mathbf{A}]\mathbf{y}^n, \mathbf{y}^n\rangle$$
$$= 0.5(\langle\mathbf{e}^{n-0.5}, \mathbf{e}^{n-0.5}\rangle + \langle\mathbf{h}^n, \mathbf{h}^{n-1}\rangle). \tag{5}$$

If the right-hand side vanishes, then the scheme is energy conserving $E_{\mathrm{E/M}}^n = E_{\mathrm{E/M}}^0$.

Scheme (4) is widely used in electromagnetic modeling. However, the FDTD algorithm causes non-physical dispersion of the simulated waves in a free-space computational lattice.

Why is zero dispersion for a special direction important? Unlike plasma problems, the charged particles in accelerators are organized and a direction of motion (the longitudinal direction) can be identified. Hence, the computational domain is very long in the longitudinal direction and relatively short in the transverse plane. Additionally, the electromagnetic field changes very fast in the direction of motion but is relatively smooth in the transverse plane.

To find the scheme, let us consider Fig. 1 and subdue an update procedure to the motion of the bunch. We suggest that a charged particle is moving in the z-direction with velocity of light. Additionally, let us suggest that our numerical scheme allows to take a time step $\Delta\tau$ equal to the mesh step Δz in the z-direction. If at the time τ_0 the particle has the position aligned with the left z-facet of the primary grid (see Fig. 1), then in the time $\tau_0 + 0.5\Delta\tau$, it will be aligned with the left z-facet of the dual grid and in the time $\tau_0 + \Delta\tau$, it will be again aligned with the next z-facet of the primary grid. It suggests that we should replace the E/M time splitting of the field components in scheme (4) by a more adequate TE/TM splitting. Indeed, in the time τ_0, it is reasonable to update the TM components $\mathbf{e}_x, \mathbf{e}_y, \mathbf{h}_z$ and the half time step later, namely in time $\tau_0 + 0.5\Delta\tau$, we have to update the TE components $\mathbf{h}_x, \mathbf{h}_y, \mathbf{e}_z$.

Following the above consideration, let us rewrite scheme (4) in the equivalent form:

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{u} = \mathbf{D}_{11}\mathbf{u} + \mathbf{D}_{12}\mathbf{v} + \mathbf{j}_u,$$
$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{v} = \mathbf{D}_{22}\mathbf{v} - \mathbf{D}_{12}^*\mathbf{u} + \mathbf{j}_v \tag{6}$$

where $\mathbf{u} = (\mathbf{h}_y, \mathbf{h}_y, \mathbf{e}_z)^{\mathrm{T}}$ and $\mathbf{v} = (\mathbf{e}_x, \mathbf{e}_y, \mathbf{h}_z)^{\mathrm{T}}$.

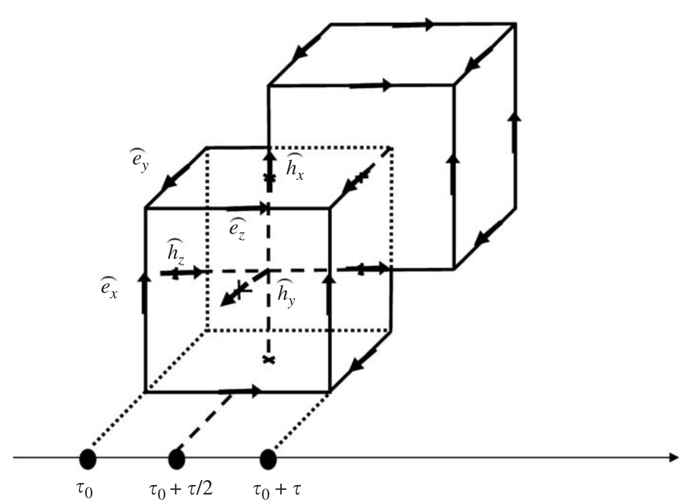

Fig. 1. Positions of the relativistic charged particle in the FIT grid in different moments of time. The time step is chosen equal to the longitudinal mesh step.