# NUMERICAL DISPERSION ERROR REDUCTION IN EM-CALCULATIONS FOR ACCELERATORS\*

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#### Abstract

In this contribution two recently proposed numerical schemes with no dispersion along the beam axis for the simulation of ultra-short, relativistic bunches are investigated. This property is of particular interest in the computation of electromagnetic wakes in linear accelerators. The numerical results obtained by both schemes are benchmarked against the analytical solution for an electron bunch moving within a cylindrical pipe with perfectly conducting walls. As a more realistic application, the longitudinal wake potential of a single bunch passing through several cells of the TESLA-FEL.

## **INTRODUCTION**

Linear accelerators used as FEL injectors constitute the cutting edge of modern electron accelerator technology. Currents above 10kA in ultra-relativistic, extremely short electron bunches of length below  $100\mu$ m can already be achieved, e.g., at the TESLA-FEL facility at DESY, Hamburg (cf. [5]). The short range wake fields produced by these bunches extend far into the THz range, i.e., they may initiate Cooper pair breakup in superconducting RF-cavities. Also the increase of single bunch energy spread and beam emittance due to the bunch wakes remains an issue, even in the ultra-relativistic regime.

In order to reveal the inner structure of field-particle interactions, numerical simulation codes are used as a standard tool in accelerator physics. In the simulation of ultrashort relativistic bunches, however, special care must be taken regarding the specific capabilities and the accuracy of the numerical method employed. The most severe problem arising in such simulations is the large numerical dispersion error in the electromagnetic field computation. The sources of dispersion errors in simulation codes based on discrete models are twofold. First, the resolution of the extremely short wave lengths in the vicinity of the bunch requires a large computational effort, which often exceeds the resources provided by today's computers. Second, most of the standard techniques for the solution of Maxwell equations exhibit an inherent numerical dispersion for high frequency waves propagating in certain directions in space. In particular, it has been shown that, for Cartesian griddiscretization, the dispersion error of the Yee-method attains its maximum in directions parallel to the coordinate axes. In the simulation of short relativistic bunches, this kind of error becomes unacceptably large, since longitudinal waves are additionally shifted by Lorentz contraction toward higher frequencies. The dispersion free computation of longitudinal wakes along the beam line remains, therefore, a major computational challenge.

In this paper we investigate two recently proposed approaches which completely eliminate the longitudinal dispersion error in the electromagnetic field computation. Instead of modifying the stencil of the spatial discretization, increasing the order of discretization accuracy or adapting the orientation of the computational mesh, the methods used here, introduce a splitted time step scheme in the update equations, which maintains the simple structure and efficiency of the spatial discretization used with the Finite-Integration-Theory (FIT)[1].

# **DESCRIPTION OF THE ALGORITHMS**

The idea of using transversal-longitudinal splitting for minimizing the longitudinal dispersion errors in combination with a moving mesh technique for wake field computations was pioneered by Novokhatski (see [3] and references therein). The two schemes discussed below, however, remain completely in the framework of the FIT. Here, the spatial discretization is defined by a primal-dual grid complex,  $(G, \tilde{G})$ . On G, the electric field is represented by electric voltages,  $\widehat{\mathbf{e}}$ , and on G the magnetic field is represented by the magnetic voltages  $\hat{\mathbf{h}}$ . The discrete counterparts of the curl-operator on G and  $\tilde{G}$  are given by the topological operators C and C, respectively. Additionally, discrete material operators,  $\mathbf{M}_{\varepsilon}$  and  $\mathbf{M}_{\mu}$ , are defined, accounting for the electrical and magnetical properties of materials in the computational domain. For further details, especially for the matrix notation applied in this work, the reader is referred to [1].

To begin with, the second order accurate, explicit Longitudinal-Transversal-Leap-Frog (LTLF) scheme is discussed. Denoting by  $\Delta t$  the time step,  $t^{(n)} = \Delta t n$  the n-th time level, the time update scheme takes the form:

$$\begin{pmatrix} \widehat{\mathbf{h}}^{(n+1)} \\ \widehat{\mathbf{e}}^{(n+1)} \end{pmatrix} = \mathbf{A}_{\mathrm{S}} \begin{pmatrix} \widehat{\mathbf{h}}^{(n)} \\ \widehat{\mathbf{e}}^{(n)} + \frac{\Delta t}{2} \mathbf{M}_{\varepsilon}^{-1} \widehat{\mathbf{j}}^{(n)} \end{pmatrix} + \frac{\Delta t}{2} \begin{pmatrix} 0 \\ \mathbf{M}_{\varepsilon}^{-1} \widehat{\mathbf{j}}^{(n+1)} \end{pmatrix}.$$

The update matrix,  $A_{\rm S}$ , is written as a product,

$$\mathbf{A}_{\mathrm{S}}(\Delta t) = \mathbf{A}_{\mathrm{T}}\left(\frac{\Delta t}{2}\right) \mathbf{A}_{\mathrm{L}}(\Delta t) \mathbf{A}_{\mathrm{T}}\left(\frac{\Delta t}{2}\right), \qquad (1)$$

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where the operators  $A_L$  and  $A_T$ , represent the update of a subsystem in transversal and longitudinal direction, respectively. This type of directional separation of the update matrix  $A_S$  is equivalent to a second order accurate Strangtype operator splitting. Each of the directional operators,  $A_L$  and  $A_T$ , is numerically equivalent to a second order accurate two-step Leap-Frog update

$$\begin{split} \mathbf{A}_{\mathrm{L/T}}(\Delta t) &= \mathbf{U}_{\mathrm{L/T}}\left(\frac{\Delta t}{2}\right) \mathbf{V}_{\mathrm{L/T}}(\Delta t) \mathbf{U}_{\mathrm{L/T}}\left(\frac{\Delta t}{2}\right),\\ \mathbf{U}_{\mathrm{L/T}}(\Delta t) &= \begin{pmatrix} 1 & -\Delta t \mathbf{M}_{\mu}^{-1} \mathbf{C}_{L/T} \\ 0 & 1 \end{pmatrix},\\ \mathbf{V}_{\mathrm{L/T}}(\Delta t) &= \begin{pmatrix} 1 & 0 \\ \Delta t \mathbf{M}_{\varepsilon}^{-1} \widetilde{\mathbf{C}}_{L/T} & 1 \end{pmatrix}. \end{split}$$

Omitting the details of a lengthy calculation, the numerical dispersion relation of the LTLF scheme, for a homogenous mesh with mesh spacing  $\Delta$  and Courant number  $\sigma = c_0 \Delta t / \Delta$ , is found to

$$A = \sigma^{2} \left( B + C - \frac{\sigma^{2}}{4} C \left( 4B + C \left( 1 - \sigma^{2}B \right) \right) \right), \quad (2)$$
$$A = \sin^{2} \left( \frac{\Delta t \omega}{2} \right), \quad B = \sin^{2} \left( \frac{\Delta k_{z}}{2} \right),$$
$$C = \sin^{2} \left( \frac{\Delta k_{x}}{2} \right) + \sin^{2} \left( \frac{\Delta k_{y}}{2} \right).$$

From (2) it follows that, for waves propagating in the longitudinal direction ( $k_x = k_y = 0$ ) and for  $\sigma = 1$ , the exact dispersion relation is recovered. Thus, for those waves no numerical dispersion is produced by the scheme. The dispersion behavior of the scheme for waves propagating in directions other than the longitudinal is shown in Fig. 1. For an extensive description of the second scheme use in this work, the TE/TM algorithm, the reader is referred to [2]. Here, we only note that TE/TM is based on an economic implicit formulation as opposed to the explicit update in (1). For a time step equal to the longitudinal mesh step ( $\sigma = 1$ ), both algorithms, TE/TM and LTLF, allow the application of a moving mesh in longitudinal direction without any need of grid-to-grid interpolation of the field quantities. In both cases, the moving mesh procedure relies on the fact that, for this special choice of the time step, the numerical and physical domain of dependence for longitudinal propagating waves coincide. The possibility of employing moving meshes, makes both algorithms particularly attractive in the computation of short range wake potentials in LINAC structures (cf. [4]).

#### NUMERICAL RESULTS

In order to demonstrate the accuracy of the two schemes, the electromagnetic field of a line charge of length  $\Delta$ , flying with the speed of light along the axis of a cylindrical pipe of radius 4 cm is numerically computed. An excitation of this form is the discrete representation of the motion of an ultra-relativistic point charge. It excites all wavelengths in



Figure 1: Phase velocity at stability limit in the x-z-plane for LTLF and Yee, respectively.

the discrete system, thus, any numerical dispersion error in the longitudinal direction would become visible in the simulation as spurious oscillation in the field solution. The analytical solution is given by,

$$\vec{E} = \frac{q}{2\pi\epsilon_0 r} \prod \left( z - c_0 t \right) \hat{\mathbf{e}}_r,$$

where the line charge distribution is,

$$\Pi(z) = \begin{cases} 1/\Delta & \text{for } |z| \le \Delta/2, \\ 0 & \text{otherwise.} \end{cases}$$

Figures 2-4 show the results of the numerical simulation. All shown field components are normalized to the radial electric field of the analytical solution at a distance 2cm away from the beam axes and the z-coordinate is given relative to the moving mesh. The radial components of the electric field after the particle has traveled the distance of 1m in the pipe is shown in Fig. 2. The absence of any numerical dispersion in the longitudinal direction is seen by the concentration of the electric field on a single grid point in the longitudinal direction. This behavior of the numerical solution accurately approaches that of the deltadistribution in the continuous case. In Fig. 3, the radial electric field component in transversal direction is shown. Both schemes show an excellent agreement with the analytical solution. With the computation of longitudinal wakes in mind, it is interesting to observe that the vanishing longitudinal component of the electric field very closely approximates by both numerical schemes (see Fig. 4).

## WAKE FIELD COMPUTATIONS

A more demanding application of the code is the wake field computation of an electron bunch in an accelerating structure consisting of 20 TESLA-cells (cf. [5]). Contrary to the test problem of the previous section, a particle moving with the speed of light within such a structure does produce a nonvanishing longitudinal wake field. The reader is referred to [2] for further details of the numerical setup



Figure 2: The radial component of the electric field after 1m distance is plotted vs. longitudinal position. The numerical solutions of the LTLF and TE/TM are concentrated on a single grid point (the position of the point charge).



Figure 3: The radial component of the electric field vs. the x-coordinate compared to the analytical solution is shown.

and application of the TE/TM scheme for this structure. Fig. 5 shows the longitudinal wake potential, computed for a Gaussian bunch of rms-width 1mm using a mesh step of 0.4mm in the longitudinal direction. Additionally, the wake potential obtained with the standard Yee scheme is given.



Figure 4: Normalized error of the longitudinal electric field component on the axis vs. longitudinal distance for the LTLF and TE/TM methods.



Figure 5: Wake potential calculated by the TE/TM, LTLF and the 2D Yee (4 times finer mesh) method for the 20 TESLA-cells structure.

Obviously, TE/TM and LTLF provide by far the most accurate results. In particular, the oscillations in the wake potential caused by the longitudinal dispersion error completely disappear for those schemes. The small difference observed between the TE/TM and LTLF curves is probably due to the more accurate Uniformly-Stable-Conformal (USC) spatial discretization of the boundaries used in the TE/TM scheme (see [2]).

# CONCLUSIONS

Two numerical algorithms for the solution of Maxwell's Equations have been investigated for their application in accelerator physics. For the analytic test problem both algorithms give very accurate results. A slight difference was observed in the calculation of the longitudinal wake potential for the TESLA RF-structure. Both schemes allow for an accurate computation of the wake potentials in complex geometry. A slightly higher accuracy is obtained with the TE/TM scheme, probably due to the USC discretization which is currently not available with LTLF.

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