WAKEFIELD COMPUTATIONS WITH THE PBCI CODE USING A NON-SPLIT FINITE VOLUME METHOD*

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Abstract

We report on a new numerical technique for the computation of geometrical wakes in three-dimensional LINAC structures. The method utilises an explicit Finite-Volume Time-Domain (FVTD) formulation. The numerical dispersion in all three axial directions is completely eliminated by choice of an appropriate staggering of the field components on the grid. Thus, contrary to most of the previously reported techniques no splitting of the time-evolution operator is necessary. This results in large savings in computational time as well as in an improved numerical accuracy. We have implemented this new technique in the PBCI code and present some preliminary results.

INTRODUCTION

Future accelerator projects require high quality beams with ultra short bunches. For the design of those projects an accurate numerical prediction of the short range wake fields in the different components of the accelerator is necessary. Typical accelerator structures are, however, several orders of magnitude longer than the size of electron bunches. The standard finite-difference time-domain (FDTD) method would require a huge amount of computational resources for the numerical solution of the problem. For this reason, the Parallel Beam Cavity Interaction (PBCI) code has been developed at TEMF for dedicated short range wake field simulations [1].

Key elements of PBCI are the application of a moving window approach in combination with a Longitudinal-Transversal operator splitting (LTLF) technique for the Finite Integration Technique (FIT) [4]. LTLF features no numerical dispersion in the direction of bunch propagation [2]. The scheme, however, suffers under the separate application of longitudinal and transverse update operators. This makes the calculations comparatively expensive. In addition, it adds an additional numerical dispersion error in the transversal directions. This motivates the present investigation of computationally less expensive, dispersion-free methods which are not based on operator splitting.

FINITE VOLUME DISCRETIZATION

Denoting by $\vec{E}$, $\vec{H}$, $\vec{J}$ and ϱ the electric and magnetic field, current and charge density, respectively, the volume integral form of Maxwell's equations for non-dispersive media with permittivity ε and permeability μ reads [3]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \epsilon\vec{E}\,\mathrm{d}V = \int_{\partial V} \mathrm{d}\vec{A}\times\vec{H} - \int_V \vec{J}\,\mathrm{d}V, \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \mu\vec{H}\,\mathrm{d}V = -\int_{\partial V} \mathrm{d}\vec{A}\times\vec{E}, \tag{2}$$

$$\int_{\partial V} \mathrm{d}\vec{A}\cdot\epsilon\vec{E} = \int_V \varrho\,\mathrm{d}V, \tag{3}$$

$$\int_{\partial V} \mathrm{d}\vec{A}\cdot\mu\vec{H} = 0. \tag{4}$$

The above integral formulation of Maxwell's equations is the starting point of Finite-Volume-type methods. In the following, Maxwell's equations are discretized on a Cartesian grid G. Traditional FVTD methods [5] allocate all Degrees of Freedom (DoF) in the same control volume of G. Contrary, the proposed scheme assigns the DoFs for each component of the electric and magnetic field strengths, current and charge density to different control volumes V_x, V_y, V_z and $\tilde{V}$ on G. Figure 1 shows the relation between the used control volumes and the "'usual"'cell volume in G. Additionally, the field and source DoFs associated with each of the control volumes are shown in the figure.

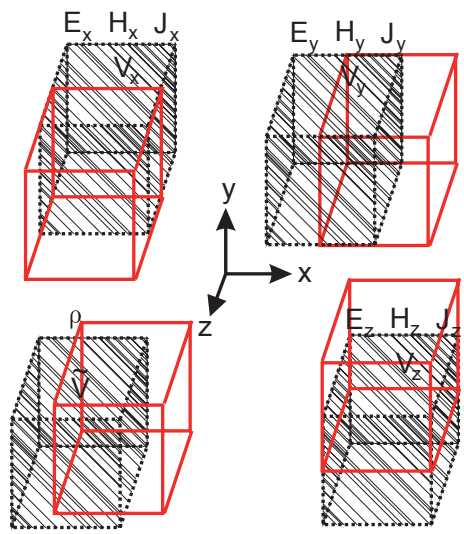

Figure 1: Control volumes (shaded) and the DoFs associated with them with respect to a cell volume in G (red).

Assuming constant field components within the respective control volumes, discrete versions of Faraday's (2),

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Ampere's (1) and Gauss's (3) laws can be constructed. The derivation of of the discrete Faraday's law is sketched in Fig. 2. According to (2) the volume integral of $\frac{\mathrm{d}}{\mathrm{d}t}\mu H_x$ is determined by the integral over the areas (shown in red) of the control volume V_x. Due to choice of field staggering, the relevant electric field components on these areas are uniquely known, so that the integrals are readily evaluated. The other field components in Faraday's law are treated in the same manner. The spatial discretization of the obtained scheme is of second order on a homogeneous and of first order accuracy on an inhomogeneous Cartesian grid.

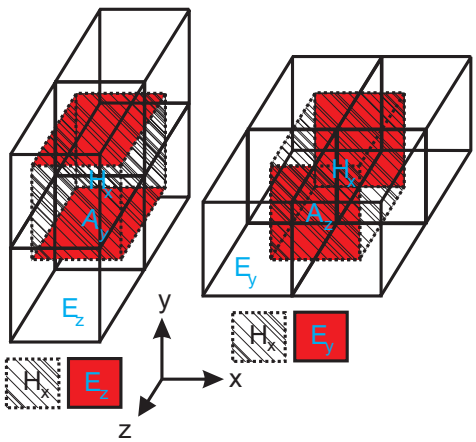

Figure 2: Calculation of $\frac{\mathrm{d}}{\mathrm{d}t}\mu H_x$ (shaded volume V_x) in the discrete Faraday's law using the values of E_y and E_z on the staggered red areas, A_z and A_y.

MATRIX FORMULATION

Collecting the field and source DoFs within each control volume into the vectors $\boldsymbol{e}$, $\boldsymbol{h}$ and $\boldsymbol{j}$, respectively, the discrete FV version of Maxwell's equations is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{M}_\epsilon \boldsymbol{e} = \boldsymbol{C}\boldsymbol{h} - \boldsymbol{V}\boldsymbol{j} \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{M}_\mu \boldsymbol{h} = -\boldsymbol{C}\boldsymbol{e} \tag{6}$$

$$\boldsymbol{S}\boldsymbol{M}_\epsilon \boldsymbol{e} = \tilde{\boldsymbol{V}}\boldsymbol{\varrho} \tag{7}$$

$$\boldsymbol{S}\boldsymbol{M}_\mu \boldsymbol{h} = \boldsymbol{0}\,. \tag{8}$$

$\boldsymbol{M}_\epsilon$, $\boldsymbol{M}_\mu$, $\boldsymbol{V}$ and $\tilde{\boldsymbol{V}}$ are symmetric and positive definite material matrices. These operators depend on the grid metrics as well as on the local material parameters ε and μ. A discrete curl is defined by the symmetric matrix $\boldsymbol{C}$ and the discrete divergence is denoted by $\boldsymbol{S}$. In analogy to their continuous counterparts the identity $\boldsymbol{S}\boldsymbol{C} = 0$ can be shown to hold [6]. Thus, the matrix formulation of the scheme builds upon a discrete vector analytical operator calculus which is very similar to the FIT [4].

TIME INTEGRATION

For numerical integration the time is discretized with time step Δt by $t^{(n)} = t^{(0)} + n\Delta t$. Denoting with $\boldsymbol{e}^{(n)}$ and $\boldsymbol{h}^{(n)}$ the discrete electric and magnetic field DoFs sampled at the time instance $t^{(n)}$ the discrete Faraday and Ampere's law are discretized in time by the Verlet-Leap-Frog (VLF) integrator:

$$\boldsymbol{h}^{(*)} = \boldsymbol{h}^{(n)} - \frac{\Delta t}{2}\boldsymbol{M}_\mu^{-1}\boldsymbol{C}\boldsymbol{e}^{(n)},$$

$$\boldsymbol{e}^{(n+1)} = \boldsymbol{e}^{(n)} + \Delta t \boldsymbol{M}_\epsilon^{-1}\boldsymbol{C}\left(\boldsymbol{h}^{(*)} - \boldsymbol{V}\boldsymbol{j}^{(n+1/2)}\right),$$

$$\boldsymbol{h}^{(n+1)} = \boldsymbol{h}^{(*)} - \frac{\Delta t}{2}\boldsymbol{M}_\mu^{-1}\boldsymbol{C}\boldsymbol{e}^{(n+1)}.$$

The fully time discrete scheme above is referred to Staggered Finite Volume Time Domain (SFVTD) method. In [6], the maximal stable time step of SFVTD for a homogeneous grid with grid spacing Δ, and a constant speed of light c was found to be exactly equal to the Courant number $\sigma := c\frac{\Delta t}{\Delta} = 1$.

DISPERSIONAN ANALYSIS

A numerical phase velocity as close as possible to the speed of light is important for the accurate simulation of wake fields over long distances. The low numerical dispersion property must be fulfilled over a broad range of frequencies and wave propagation directions. In this section the accuracy of SFVTD in terms of dispersion error is analysed and compared with those of the LTLF scheme and non-split FIT.

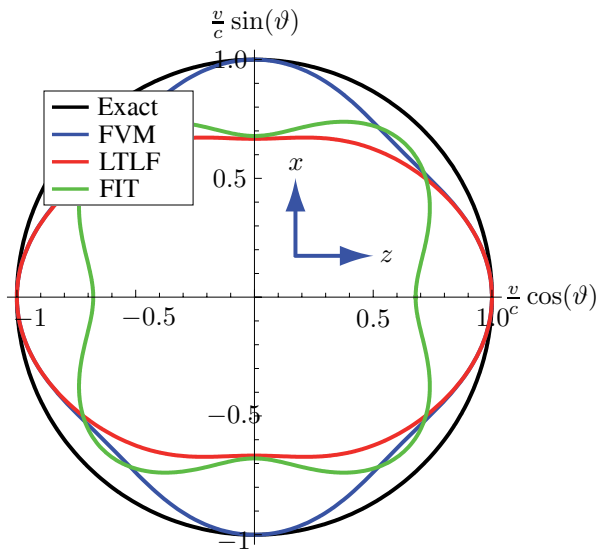

Figure 3: Directional dependence of the numerical phase velocity v for three points per wavelength in the xz-plane for LTLV, non-split FIT and the SFVTD method.

Making a plane wave solution ansatz $\exp j(\omega t - \vec{k}\cdot\vec{r})$ and using the dimensionless wave vector $\vec{\beta} = \Delta \cdot \vec{k}$ and

frequency $\tilde{\omega} = \Delta t\,\omega$, the following numerical dispersion relation for the SFVTD scheme is obtained:

$$\sin^2(\frac{\tilde{\omega}}{2}) = \sigma^2 \left(\sum_{\gamma} \sin^2(\frac{\beta_\gamma}{2}) - \frac{1}{2} \sum_{\gamma \neq \delta} \sin^2(\frac{\beta_\gamma}{2}) \sin^2(\frac{\beta_\delta}{2}) \right)$$
$$\gamma, \delta \in \{x, y, z\}\,. \qquad (9)$$

From (9) the numerical phase velocity $v = c\tilde{\omega}/\beta$ is calculated. Figure 3 shows v/c for a resolution of three points per wavelength on the xz-plane. The phase velocity for each of the schemes is evaluated at the respective stability limit. The exact phase velocity $v = c$ is never approached by FIT, the LTLF method approaches it along the z-axis and the SFVTD method approaches it along the x- and z-axis. Also in between those exact cases, the SFVTD method is superior to the LTLF scheme and in a large region also to the non-split FIT. Fig. 4 shows the behaviour of the phase error in 3D. It is clearly seen that SFVTD approaches its minimal error along the coordinate axis, in contrast to the FIT which has an optimum dispersion characteristics along the diagonal directions.

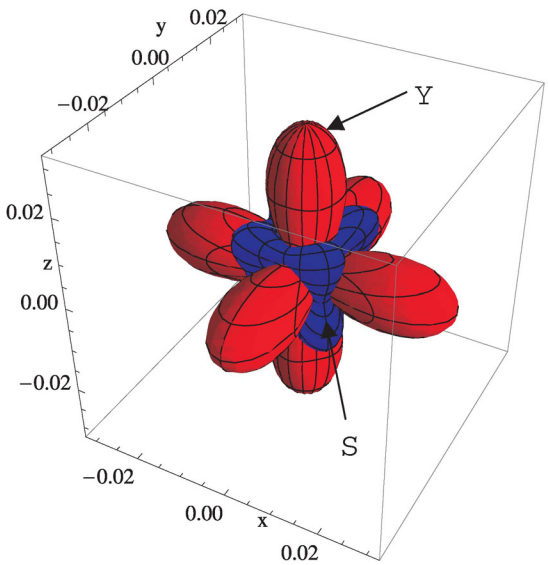

Figure 4: Directional dependence of the error in the numerical phase velocity v for three points per wavelength for FIT and the proposed SFVTD scheme.

NUMERICAL VALIDATION

As a validation test the longitudinal wake potential of a Gaussian line bunch with $\beta = 1$ and $\sigma_z = 0.02\mathrm{cm}$ passing a closed pill box cavity on the axis is numerically calculated. The cavity has a gap length of $10\mathrm{cm}$ and a radius $5\mathrm{cm}$. For the numerical solution of the problem, the presented SFVTD method was applied on a moving mesh. The results are compared with the analytical solution [7] for a Gaussian bunch ($\sigma_z = 0.02\mathrm{cm}$) [7]. Figure 5 shows the

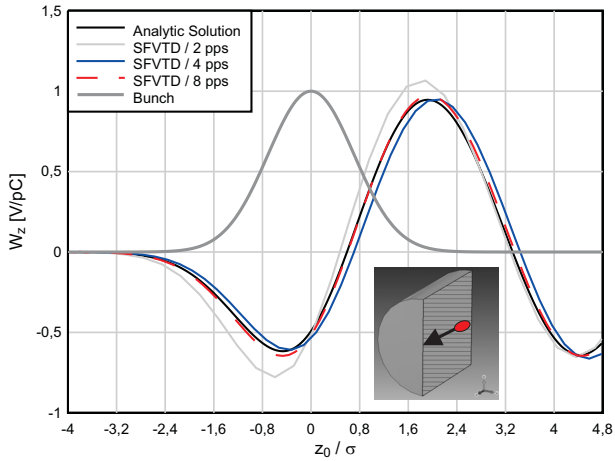

Figure 5: Comparison of the analytical solution (black) of the longitudinal wake field W_z inside a pill box cavity with the numerical solution obtained by the SFVTD method for three different grids.

fast numerical convergence toward the analytical solution for different number of points per sigma (pps).

CONCLUSIONS

A non-split SFVTD with no numerical dispersion along the coordinate axes has been presented. It has been theoretically demonstrated that the method has better numerical dispersion properties in comparison to LTLF and the non-split FIT. The numerical validation example shows, that the method is capable for accurate short range wake field computations in accelerator structures.

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