

# COMPUTATION OF ELECTROMAGNETIC FIELDS GENERATED BY RELATIVISTIC BEAMS IN COMPLICATED STRUCTURES

Igor Zagorodnov\*, Deutsches Elektronen-Synchrotron, Hamburg, Germany

## Abstract

We discuss numerical methods for computation of wake fields excited by short bunches in accelerators. The numerical methods to implement a low-dispersive scheme, conformal approximation of the boundaries, surface conductivity, and indirect wake potential integration are reviewed. The implementations of these methods in electromagnetic code ECHO for 2D and 3D problems are presented. Several examples of application of the code to important problems in the European Free Electron Laser project and in the Linac Coherent Light Source (LCLS) project are considered.

## INTRODUCTION

This paper gives an overview of our research in numerical methods for electrodynamics and accelerator physics. It presents original low-dispersive numerical methods (TE/TM implicit and explicit schemes) for calculation of electromagnetic fields in accelerators. The developed algorithms allow for calculation of electromagnetic fields of ultra-short bunches in very long structures. In order to reduce the numerical errors the Uniformly Stable Conformal (USC) algorithm is developed and described. It allows for a conformal geometry modeling without time step reduction. Combination of both described approaches (the low-dispersive numerical scheme and the conformal technique without time step reduction) gives high quality results even on a coarse mesh with a large time step. Indirect method for wake potential integration is reviewed. The algorithms are implemented in code ECHO which is available at [1].

## NUMERICAL METHODS

In order to simulate self-consistent dynamics of the charged particles, we need to be able to solve at least two kinds of problems: (i) to calculate the electromagnetic field for the given charges and currents and (ii) to solve equations of motion of charged particle in the given electromagnetic field. In this paper we consider the approaches to effective solution of the first problem.

### *Low-Dispersive Numerical Schemes*

The particle-in-cell (PIC) method [2] is an effective approach for simulation of beam dynamics in accelerators. In this model one emulates nature by following the motion of a large number of charged particles in their self-consistent electric and magnetic fields. The electromagnetic fields in many PIC codes are computed using the finite-difference time domain (FDTD) method [3], [4]. As any numerical mesh approach, the FDTD method suffers from an anisotropic

numerical dispersion. The numerical wave phase speed is slower than the physical one. Hence, the high energy particles can travel in vacuum faster than their own radiation. This effect is commonly referred as numerical Cherenkov radiation [5], which (due to its accumulative character) corrupts the simulation. Hence, the electromagnetic field computation for short relativistic bunches in long structures remains a challenging problem even with the fastest computers.

Several approaches [5]- [9] have been proposed to reduce the accumulated dispersion error of large-scale three-dimensional simulations for all angles and for a given frequency range. These methods require the usage of larger spatial stencils and a special treatment of the material interfaces. The increased computational burden justifies itself for computational domains large in all three dimensions. However, in the accelerator applications the domain of interest is very long in the longitudinal direction and relatively narrow in the transverse plane. Additionally, the electromagnetic field changes very fast in the direction of bunch motion but is relatively smooth in the transverse plane. Hence, it is extremely important to eliminate the dispersion error in the longitudinal direction for all frequencies. If the numerical dispersion is suppressed then a quite coarse mesh and moderate computational resources can be used to reach accurate results. It was shown in wake field calculations by A. Novokhatski [10] and in plasma simulations by A. Pukhov [11].

As it is well known, the FDTD method at the Courant limit is dispersion free along the grid diagonals and this property can be used effectively in numerical simulations [12]. However, the only reasonable choice in this case is to take equal mesh steps in all three directions. Alternatively, a semi-implicit numerical scheme without dispersion in the longitudinal direction with a simpler conformal treatment of material interfaces and the usage of non-equidistant grids has been developed in [13]- [15].

The scheme described in [10, 14] allows to solve the scalar problem and to calculate the wake potential for fully axially symmetric problems with staircase approximation of the boundary. In [15], a three-level scheme  $\mathbf{R}(\mathbf{y}^{n+1} - 2\mathbf{y}^n + \mathbf{y}^{n-1}) + \mathbf{A}\mathbf{y}^n = \mathbf{f}^n$  for the vectorial problem was suggested. Our scheme is based on a second order hyperbolic wave equation for vector potential. A modification of the USC method [16] is used to avoid the "staircase" problem and to obtain a second order convergent algorithm. However, the operator  $\mathbf{R}$  in this scheme is not self-conjugate; and therefore an "energy" conservation cannot be proven theoretically by the standard techniques [17]. Additionally, the scheme is not economical for general three-dimensional geometries. The last drawback can be overcome by splitting methods [17]. However, the absence of a theoretical proof

\* Igor.Zagorodnov@desy.de

for an energy conservation has stimulated us to look for an alternative approach in the three-dimensional case.

In paper [18], a new two-level implicit economical conservative scheme for electromagnetic field calculations 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 [15], the new method is based on a TE/TM-like splitting of the field components in time. Additionally, it uses an alternating direction splitting of the transverse space operator that renders the scheme computationally as effective as the conventional FDTD method. Unlike the FDTD ADI [19] and low-order Strang [20] methods, the splitting error in our scheme is only of fourth order. The new scheme assures energy and charge conservation. Additionally, the usage of damping terms allows suppressing a high frequency noise generated due to the transverse dispersion and current fluctuations. The dispersion relation of the damping scheme is derived and analysed. Numerical examples show that the new scheme is much more accurate in long-time simulations than the conventional FDTD approach. For axially symmetric geometries, the new scheme performs two times faster than the scheme suggested in [15].

Other methods have been developed in [21, 22]. However, all these approaches loose in simplicity, efficiency and memory demands compared to Yee's scheme [3]. In paper [23] we present a scheme which competes with Yee's algorithm. The scheme does not have dispersion in the axis direction. It is based on a TE/TM-like splitting of the field components in time. It is simpler and faster than the implicit version, introduced earlier in [18]. The numerical effort is scaled as 5/3 compared to Yee's algorithm for the same time step. But the explicit scheme allows for a larger time step than Yee's algorithm. With such choice the explicit TE/TM scheme requires only 18% more computational time, while the memory demands remain the same. The explicit character of the new scheme allows for USC method (see next section) to reach the second order convergence and the scheme can be parallelized easily. A version of this explicit scheme for rotationally symmetric structures is free from the progressive time step reducing for higher order azimuthal modes as it takes place for conventional Yee's FDTD method used in the most popular accelerator codes [24, 25].

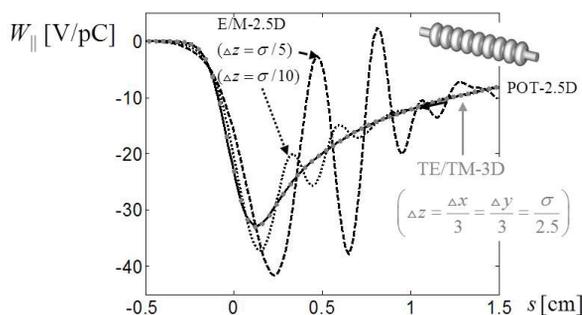


Figure 1: Wake potentials obtained by different methods.

As an example we consider a structure consisting of the 20 TESLA cells bounded by infinite ingoing and outgoing pipes. Fig. 1 shows the longitudinal wake potential

$$W_{||}(x, y, s) = Q^{-1} \int_{-\infty}^{\infty} [E_z(x, y, z, t)]_{t=(z-s)/c} dz, \quad (1)$$

for a Gaussian bunch with an RMS length  $\sigma = 1$  mm moving on the axis. The solid line (POT-2.5D) corresponds to the reference solution obtained with the vector potential method [15]. The two other lines show results obtained with different mesh resolutions from the TBCI code [25] based on the classical Yee's scheme (E/M-2.5D). The oscillations that appear are due to the dispersion error of Yee's scheme. The gray points represent the result obtained by the three-dimensional TE/TM scheme. It can be seen that the three-dimensional TE/TM scheme produces very accurate results even on the coarse mesh. Indeed, the three-dimensional code uses only 2.5 mesh points per  $\sigma$  in the longitudinal direction. In the transverse direction the mesh steps are even three times larger.

### Conformal Mesh Methods

In the past decades most of the research on FDTD has been focused on overcoming the staircase problem [26] of the conventional algorithm. These attempts have resulted in the development of various modified versions of FDTD. However, many of these approaches require a complicated distorted-mesh information and demand to reduce the time step due to the reduction of the effective mesh step sizes near the boundary. In [27, 28] two Conformal FDTD algorithms without time step reduction have been introduced. In some cases they have a better accuracy than the conventional staircase approach, but the convergence remains of first order. Another approach based on interpolation of the fields has been introduced in [29]. The algorithm is second order convergent, but a generalization to 3D is not straightforward. In [30] a Fictitious Domain approach is described, which also has only first order convergence.

In paper [16] we have introduced a new stable second order convergent algorithm on Cartesian grids without time step reduction, Uniformly Stable Conformal (USC) method. Our algorithm is introduced in context of the Finite Integration Technique [31] and is based on the Partially Filled Cells (PFC) scheme [32, 33]. The USC method is a new stable second order convergent algorithm on Cartesian grid.

The main drawback of the USC algorithm is the usage of extended stencils near to the boundary (exploiting of non-diagonal material matrices). Motivated by the need for a simplification of USC, both in terms of implementation effort and intuitive understanding, we present in [34] a new Simplified Conformal (SC) scheme. It does not use extended stencils, but at the same time it remains accurate and stable without time step reduction. The new scheme is not second order convergent for general geometries. However, it is much more accurate than the "staircase" method. Numerical tests show a second order convergence of the new scheme

on moderate meshes. Hence, as our experience shows, in practical examples the scheme has the same level of accuracy as the more complicated USC method. Like the USC scheme the new method is a fully three-dimensional technique, with a much simpler realization. The convergence of the algorithm without the need to reduce the time step is analyzed on several numerical examples in two and three dimensions.

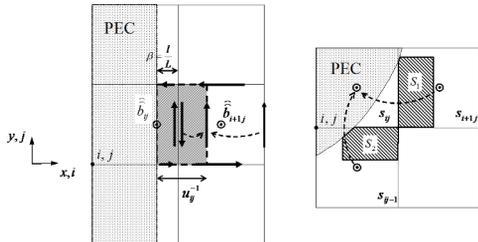


Figure 2: Geometric interpretation of weighting procedure.

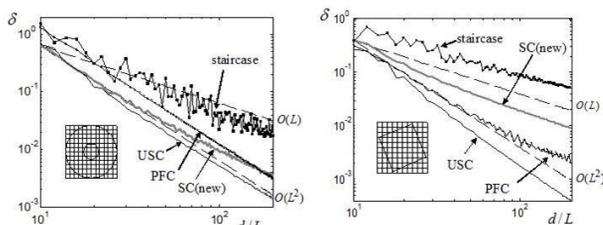


Figure 3: Convergence of different methods.

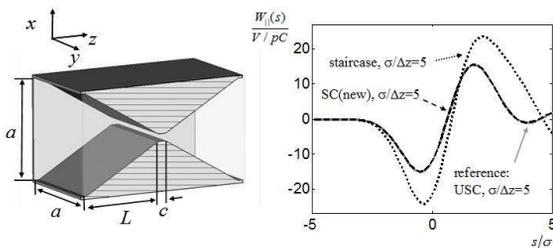


Figure 4: Longitudinal wake potential of tapered collimator.

SC scheme. The convergence of PFC scheme [33] is shown by a line with circles, and for the staircase approximation it is shown by line with squares. As we can see the new SC scheme shows very accurate results and near second order convergence. Fig. 3(right) shows a more stringent test: a perfectly conducting square rotated by the angle relative to the x-axis. The magnetic field of the TE mode is compared to the numerical solution after a period of time  $T = c^{-1}d/\sqrt{2}$ , where  $d$  is the diagonal of the square. Here, the SC scheme shows a first order convergence. However, the accuracy of the scheme is one order of magnitude better than of the staircase approach. In all examples the USC scheme, as expected, shows second order convergence.

Finally, we test the SC scheme on the example of a three-dimensional rectangular collimator shown in Fig. 4 (with inner aperture  $b * a$ ,  $b$  is not indicated in the figure). Again, we use the SC method with semi-implicit scheme [22] that allows to leave the longitudinal edges of the mesh as accurate as in PFC scheme and to restrict the modification only to edges in transverse plane. Fig. 4 shows the results for the monopole wake field of the relativistic Gaussian bunch moving on the axis. It compares the result of the staircase scheme to the one obtained with the new SC scheme. The geometric parameters ( $a = 38\text{mm}$ ,  $L = 103.8\text{ mm}$  and  $c = 0.4\text{ mm}$ ,  $b = 1.4\text{mm}$ ) describe one of the collimators used in experiments at SLAC. With only 5 points per bunch length  $\sigma = 1\text{mm}$ , the new SC scheme gives much more accurate result than the staircase scheme.

### Indirect Methods for Wake Potential Integration

For short bunches, a long-time propagation of the electromagnetic field in the outgoing vacuum chamber is required to take into account the scattered fields which will reach the bunch at later times. To drastically reduce the computational time and avoid numerical error accumulation, several indirect integration algorithms were developed for rotationally symmetric geometries [35]- [38].

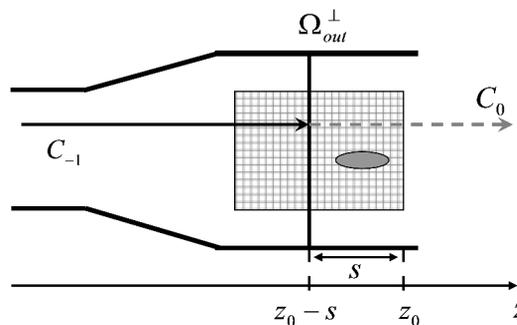


Figure 5: Contour  $C_{-1}$  for direct integration and cross-section  $\Omega_{out}^\perp$  for indirect integration algorithm

For three-dimensional structures the indirect integration algorithm was known only for cavity-like structures [36]. Papers [39], [40] introduce a new general algorithm for the treatment of arbitrary three-dimensional structures. Several

numerical examples are presented in [39] to illustrate the accuracy and efficiency of the new method.

Paper [39] shows how to replace the improper integral in Eq.(1) by proper integral. The longitudinal wake potential can be written as

$$QW_{||}(x, y, s) = \int_{C_{-1}} [E_z(x, y, z, t)]_{t=(z-s)/c} dz + u(x, y, s),$$

where the function  $u(x, y, s)$  describes the impact of the radiated field on the bunch in the outgoing waveguide (path  $C_0$  in Fig. 5). It is proven in [39] that this function can be found from the solution of the Poisson equation in cross-section  $\Omega_{out}^+$ . The same can be done for the ingoing pipe.

The new indirect method was also used for the accurate calculation of collimator wake fields [41]. It was interesting to observe that the kick factor depends strongly on the length of the interior collimator pipe, the effect not described in the literature earlier. Note that this problem was very difficult to treat in three dimensions satisfactorily with the old techniques.

### Conductive Walls

In the following we will discuss a conformal scheme for metallic walls with finite conductivity. "Conformal" means here a better description of material interfaces in order to reduce approximation errors and to improve the convergence [16].

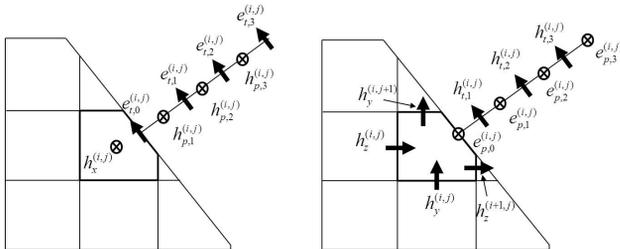


Figure 6: A boundary cell in the vacuum and 1D conductive line in the metal.

For the case of rotationally symmetric geometry and usage of the "staircase" approximation for the boundaries a similar scheme was described in [42]. However the "staircase" scheme provides only first order convergence. Attempts of authors [42] at that time to suggest and to implement a conformal scheme (with second order convergence) have failed due to instabilities of the scheme for the maximal time step required for "dispersion-free" propagation. The conformal scheme with conductivity described in [43] shows the second order convergence and the stability. We consider the case of high conductivity  $\kappa$  when only tangential components of the field propagate in the metal. For example, for the Gaussian bunch with rms length  $\sigma_z$  this condition is fulfilled if  $\kappa\sigma_z \gg \epsilon_0$ , where  $\epsilon_0$  is electric permittivity of the vacuum. It can be seen from Fig. 6 that at the boundary cells there are two tangential components of the electric field which should be updated at each time step. A detailed discussion of this

approximation and its equivalence to the surface impedance boundary condition can be found in [33], [42].

In order to obtain second order convergence and avoid time step reduction, we use conformal method with enlarged boundary cells in the same way as described in [15]. However, for the stability of the conformal scheme it was crucial to use the full interpolation scheme with eight weights [16].

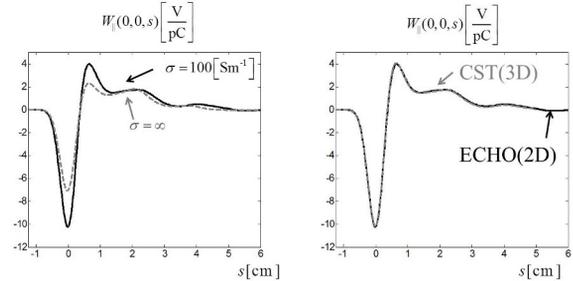


Figure 7: Longitudinal wake potential of tapered collimator.

As an example problem we consider a symmetric, tapered collimator (see Fig. 4). The dimensions are: width and height of large pipe  $a = 10$  cm, length of tapers  $L = 5$  cm; height of the minimum gap  $b = 2$  cm and  $c = 12$  cm. Code ECHO2D is capable of modeling structures with metallic walls of finite conductivity. The tapered walls and the walls of the minimum gap section are taken to have conductivity  $\sigma = 100$  S/m, while the remaining surfaces are assumed to be perfectly conducting. In the left plot of Fig. 7 we compare the longitudinal wake for this collimator with one that has the same geometry but is perfectly conducting. The Gaussian bunch in the simulations has an rms length  $\sigma_z = 0.25$  cm. Both wakes were obtained with ECHO2D. In the right plot of Fig. 7 we compare the ECHO2D wake potential with the one obtained using a fully three-dimensional, commercially available code CST [44]. The good agreement between the results indicates a good accuracy of the conformal meshing and the resistive wall modeling in ECHO2D.

## CODE ECHO

In this section we review different modules of code ECHO.

### Codes ECHOz1 and ECHOz2 for Rotationally Symmetric Geometries

The code ECHOz1 is a code optimized for fully rotationally symmetric problems (only monopole mode). It is based on second order scalar wave equation as described in [15]. The code ECHOz2 is a code optimized for rotationally symmetric geometries. It calculates any azimuthal mode for off-axis bunch. It is based on TE/TM conformal scheme with conductivity as described in [18,43]. The both codes are stand-alone Windows applications with Graphical User Interface (GUI) written in Microsoft Visual C with MFC. Code ECHOz2 can treat conductive walls.

### Code ECHO2D for Rectangular Geometry

The code ECHO2D is a code optimized for rectangular and rotationally symmetric geometries. Under rectangular geometries we mean structures having rectangular cross-section, where the height can vary as function of longitudinal coordinate but the width and side walls remain fixed. For such structures, we have derived a Fourier representation of the wake potentials through one-dimensional functions. The computation resource requirements for this approach are moderate and comparable to those for finding the wakes in 2D rotationally symmetric structures. Numerical examples obtained with the new code are presented in [43]. The code is parallelized to calculate several modes simultaneously. It is based on TE/TM conformal scheme with conductivity as described in [43]. It is a console application in C++ compiled for Windows, Linux and MAC OS. The post-processing can be done with Matlab scripts.

### Code ECHO3D for Arbitrary Geometry

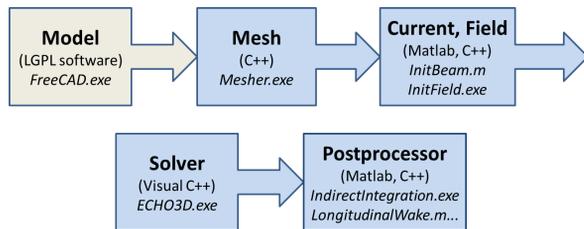


Figure 8: Workflow for ECHO3D.

Recently we have done release of code ECHO3D for arbitrary perfectly conducting geometries. The workflow diagram is shown in Fig. 8. The free source code FreeCAD [45] can be used for creating of STL description of 3D geometry. A short manual with several examples including the TESLA cavity with RF couplers can be found at [1]. The code is based on TE/TM conformal scheme. The current version is non-parallelized but we hope to implement the parallelization in the next release.

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