Computa­tion of Electromagnetic Fields Gen­er­ated by Rela­tiv­ist­ic Beams in Com­plic­ated Struc­tures

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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 Light­source (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 ac­cu­mu­la­tive 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 do­ mains 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 $R(y^{n+1} - 2y^n + y^{n-1}) + Ay^n = f^n$ 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 $R$ in this scheme is not self-con­ju­gate; and there­fore an “en­ergy” con­ser­va­tion can­not be pro­ven theo­ret­i­cally by the stand­ard tech­niques [17]. Al­tem­atively, 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

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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 lose 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].

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

$$W(x, y, s) = Q^{-1} \int_{-\infty}^{\infty} [E(z, y, z, t)]_{r = (z-s)/c} dz,$$

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 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.

![Figure 1: Wake potentials obtained by different methods.](image-url)
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. 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].

A geometric interpretation of the weights defined by the USC procedure is presented in Fig. 2 and described in details in [34]. To check the convergence of the USC and SC schemes without reduction of the time step we consider two-dimensional numerical examples: resonant oscillations in a square and a ring. In the validation examples we set an initial field in the entire calculation domain corresponding to an analytically determined eigensolution [34] and start the time stepping-procedure. After a (long enough) period of time we compare the numerical solution with the exact one. For simplicity we use a series of equidistant meshes. Our first example is a perfectly conducting ring. The magnetic field of the TE mode is compared to the numerical solution after a period of time \( T = c^{-1}a\sqrt{2} \), where \( a \) is the exterior radius of the ring. The relative error \( \delta \) of the numerical obtained magnetic field is shown in Fig. 3 by a solid black line for the USC scheme. The grey line shows results for the new

\[ \Omega_{out}^{L} \]

Figure 2: Geometric interpretation of weighting procedure.

\[ C_{-1} \]

\[ z_{0} \]

\[ S \]

\[ z \]

Figure 5: Contour \( C_{-1} \) for direct integration and cross-section \( \Omega_{out}^{L} \) 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

$$QW_{\parallel}(x, y, s) = \int_{C_1} [E_z(x, y, z, t)]_{t=(z-s)/\gamma} \, dz + u(x, y, s),$$

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].

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 $\kappa \sigma_z > \epsilon_0$, 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 6: A boundary cell in the vacuum and 1D conductive line in the metal.](image)

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.

![Figure 7: Longitudinal wake potential of tapered collimator.](image)

**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 symmetric codes.

The code ECHOz2 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 symmetric codes.
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

Recently we have done release of code ECHO3D for arbitrarily perfecting conductive 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.

REFERENCES

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