Journal of Computational Physics **148,** 125–132 (1999)
Article ID jcph.1998.6107, available online at http://www.idealibrary.com on IDEAL®

A Modified Perfectly Matched Layer Implementation for Use in Electromagnetic PIC Codes

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Received October 21, 1997; revised March 25, 1998

A modification to the Berenger perfectly matched layer (PML) absorbing boundary condition that allows it to be used in particle-in-cell applications where the primary power flow through the boundary is due to electromagnetic radiation is presented. Instead of modeling particles within the PML, a term is introduced which diffuses charge conservation errors arising from the removal of particles incident on the PML to the outer boundary. Numerical results are provided to demonstrate the performance of the algorithm. © 1999 Academic Press

INTRODUCTION

Electromagnetic particle-in-cell (PIC) codes find widespread use at Sandia National Laboratories investigating the physics of light-ion diodes [1], applied-B ion diodes [2], magnetically insulated transmission lines (MITLs) [3], and high power microwave tubes [4]. One difficulty that frequently occurs when modeling such structures is in the handling of particle flux through simulation outlet ports. Considerable research has been performed on the development of absorbing boundary conditions for the finite-difference time-domain (FDTD) method [5]. One of the more popular techniques used to address this problem has been one-way wave equations (or annihilators), such as the first- and second-order Mur [6] algorithms. This approach works well for many common types of transverse electromagnetic (TEM) transmission lines, provided the boundary is not located near a discontinuity or source where higher order modes can be present [7]. In our implementation of these outgoing boundary conditions in electromagnetic PIC codes, particles passing through these boundaries are simply removed from the simulation (“killed”). Unfortunately, the effect of the particles on the fields at the boundary is not accounted for by the boundary condition leading to errors in the field and potentially instabilities. Additionally, one-way wave equation based boundary conditions tend to be narrow band and directional so they do not perform as well in simulations that contain more general (e.g., dispersive) waveguiding structures and electromagnetic radiation.

Recently Berenger proposed the perfectly matched layer (PML) [8] which introduces an artificial, lossy layer that matches the phase velocity and impedance of the adjacent physical medium. The PML has demonstrated superior performance in a wide range of electromagnetic applications [9–12] and is attractive for many PIC applications. In contrast to Jost *et al.* [13] we have taken a simple approach which avoids the treatment of particle interactions within the PML medium. However, if we simply "kill" particles as they cross into the PML region without modifying the associated fields we will adversely affect the conservation of charge leading to DC fields and anomalous power flow through the boundary. In this paper we present a modification to the PML that attempts to diffuse the charge conservation errors associated with the removal of particles incident on the PML boundary to the outer boundary. Such a correction is suitable for applications where the particle flux through the boundary is small and the primary power flow through the boundary is due to electromagnetic radiation.

BERENGER PERFECTLY MATCHED LAYER

The Berenger PML [8, 9] splits the fields into subcomponents and introduces loss terms for the electric (σ) and magnetic (σ^*) fields to cause the decay of propagating fields. The conductivities are chosen to satisfy the matching condition

$$\frac{\sigma_i}{\epsilon_o} = \frac{\sigma_i^*}{\mu_o}, \tag{1}$$

where i indicates the direction (x, y, or z), which enforces the continuity of the wave impedance and phase velocity independent of frequency. To reduce the numerical reflections from the PML interface, due to an abrupt change in conductivity, a gradual spatial variation (typically parabolic) of the conductivities is used. Because of the rapid attenuation of waves in the PML medium exponential differencing [14] is typically used to derive the discrete form of the field update equations. In addition, the outer boundary of the PML region is typically terminated with a perfect electric conductor.

We have implemented the PML update equations in our 3D electromagnetic PIC code QUICKSILVER [15] which supports multiple blocks (conformal regions of space with separate meshes) as a new type of block. This configuration reduces the cost of the PML by incurring the additional overhead of the PML only where needed. In addition, this structure allows us to use an implicit field solve algorithm [16], which is often needed to reduce the noise associated with the locally exact charge conservation algorithm in the blocks where the physics of the particles is of primary interest. The PML and standard blocks are connected by requiring the conductivities to be zero over the cells in the connection plane of the PML block, thereby allowing the total field to be arbitrarily decomposed into the partial field components. Particles are "killed" when they cross into PML blocks analogous to our one-way wave equation outlets.

PML MODIFICATIONS FOR PIC

As noted in the Introduction, simply "killing" particles as they enter the PML region without modifying the associated fields would adversely affect the conservation of charge in the simulation. Lack of charge conservation at the PML can generate anomalous DC fields which results in a nonphysical power flow through the boundary. Simulation results could be adversely effected as the level of the nonphysical power flow approaches that of the physical power flow through the boundary. Several different approaches have been used to address the issue of charge conservation in PIC codes [17]. Another interesting approach was developed by Marder [18]. This method diffuses charge conservation errors to the simulation boundary by introducing a pseudo-current into the update of the electric field. We propose to apply this method as a first-order correction to diffuse charge conservation errors at the PML interface to the outer boundary.

To summarize the use of the pseudo-current, a scalar measure of charge conservation is defined

$$F = \nabla \cdot \mathbf{D} - \rho. \tag{2}$$

It should be noted that the only contribution to ρ in (2) within the PML region is at the interface plane. Additionally, our implementation of this correction is greatly simplified because the term F is already computed by subroutines associated with the charge conservation diagnostic in QUICKSILVER. The pseudo-current is formed by computing the gradient of F and scaling it by a constant factor d. The pseudo-current is then added to the Ampére's law terms of the PML equations. If we take the divergence of the resulting equations and substitute (2) we obtain the inhomogeneous diffusion equation:

$$\frac{\partial F}{\partial t} - d\nabla^2 F = -\left(\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} + \sigma_y \frac{\partial E_{xy}}{\partial x} + \sigma_z \frac{\partial E_{xz}}{\partial x} + \sigma_x \frac{\partial E_{yx}}{\partial y} + \sigma_z \frac{\partial E_{yz}}{\partial y} + \sigma_x \frac{\partial E_{zx}}{\partial z} + \sigma_y \frac{\partial E_{zy}}{\partial z}\right). \tag{3}$$

Observe that the last terms on the right-hand side are analogous to the divergence of the conduction current ($\sigma\mathbf{E}$) through the PML region.

The parameter d determines the rate at which F diffuses. To ensure stability we select d such that it satisfies the stability condition

$$0 \leq k = 2d\Delta t \sum_{i=1}^{N} \frac{1}{(\Delta x_i)^2} < 1, \tag{4}$$

where $N = 1$ is used for one-dimensional preferential diffusion ($\nabla F \equiv \partial F/\partial n$) in the direction normal ($\hat{\mathbf{n}}$) to the boundary or $N = 3$ for general three-dimensional diffusion. In the following example we will refer to the normalized diffusion constant k defined above.

NUMERICAL EXAMPLE

In this section we present QUICKSILVER results from two simple examples, each of which is based on the practical application that motivated the development of the PML correction but which were designed to emphasize the need for the correction as well as to demonstrate typical performance expectations and limitations.

To consider the performance of our modifications we used the parallel-plate transmission line shown in Fig. 1. The geometry was discretized using cells with a length and width of

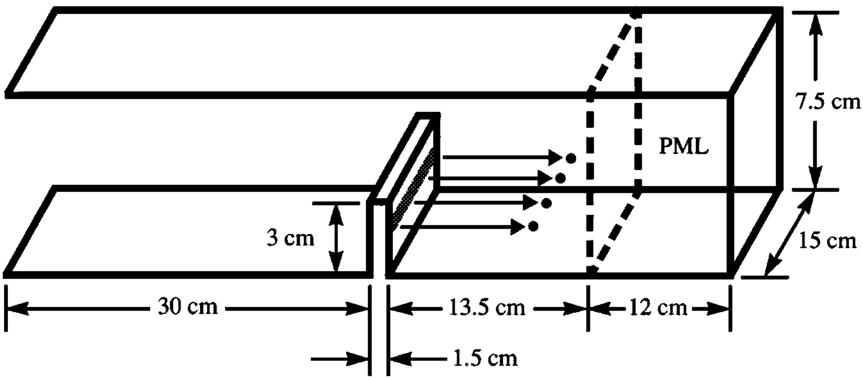

FIG. 1. Parallel-plate transmission line with iris test case geometry (not to scale).

1.5 cm and a height of 0.75 cm. A simulation time step of 18.4 ps was used. Electrons were emitted from a row of cells along the entire width of the iris at a height of three cells with a peak beam current of 100 A and a momentum (normalized by the mass) of $\gamma v = 10^{12}$ m/s, where $\gamma = 1/\sqrt{1-(v/c)^2}$, v is the velocity, and c is the speed of light in vacuum. This artificially high momentum value was chosen to minimize space-charge effects in the beam. Similar reductions in charge conservation errors were observed for more realistic values (10^8 m/s). A 1-V potential difference between the plates determined the TEM wave used to excite the parallel-plate transmission line. The Gaussian pulse used to drive both the field and beam emission had a full-width half-maximum duration of 617 ps centered at 1110 ps. The pulse parameters were chosen to excite frequencies below the cutoff of the first higher order parallel plate waveguide mode and to allow adequate resolution of the pulse shape with the simulation time step. The parameters of the PML region were chosen to provide a reflectivity on the order of 10^{-4} and resulted in an eight cell long PML block with an electric conductivity that varied parabolically from 0 to 0.27 Mho/m. Perfect magnetic conductors (mirrors) were used as boundary conditions on the side walls of the transmission line. This geometry was selected as a test case because it provided us with good control of the particle flux through the boundary. In addition, this configuration acted as a worst-case scenario because the initial practical problems of interest had a relatively low particle flux through the PML interface with a somewhat random spatial distribution. The primary measure of performance will be the conservation of charge since the adverse effects on the simulation results increase with errors in charge conservation.

In Fig. 2, we show the errors in charge conservation in the PML region for one-dimensional diffusion and several different values of the normalized diffusion constant k. As expected, due to the presence of charge only at the interface in the PML block, the major contribution to the lack of charge conservation comes from the errors in the field through the term $\nabla \cdot \mathbf{D}$. As the rate of diffusion is increased the errors are driven to zero faster. For nonzero values of k the errors eventually decay to zero. Note that for the $k = 0.1$ case the shape of the error curve is consistent with the Gaussian excitation pulse. Although not shown in a figure, when a constant beam is used for this geometry only the $k = 0.1$ case succeeds in clamping (the slope of the error curve approaches zero) the approximately linear error growth to some constant value for the same duration simulation.

In Fig. 3, we compare the performance of the one-dimensional diffusion, $N = 1$, to three-dimensional diffusion, $N = 3$, for the value $k = 0.1$. As expected, the case $N = 3$ produces

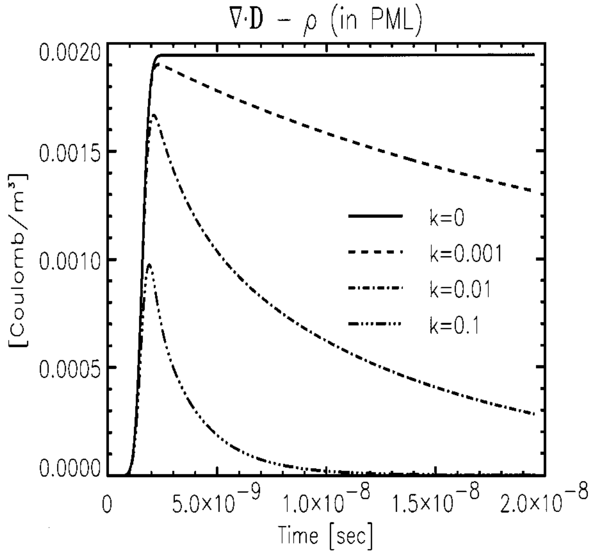

FIG. 2. Computed $\nabla \cdot \mathbf{D} - \rho$ in the PML region for one-dimensional diffusion.

a more rapid reduction of the charge conservation errors. There appears to be a slight overshoot associated with the stronger diffusion in the $N = 3$ case as the peak and late time errors are greater in the $N = 3$ case. From an implementation point of view it is easier to implement three-dimensional diffusion because no extra bookkeeping is associated with the orientation of the PML interface planes or the application of the pseudo-current term to the update of the electric field. Our present implementation uses $N = 3$ by default. It should also be noted that no stability problems have been encountered as long as (4) is satisfied.

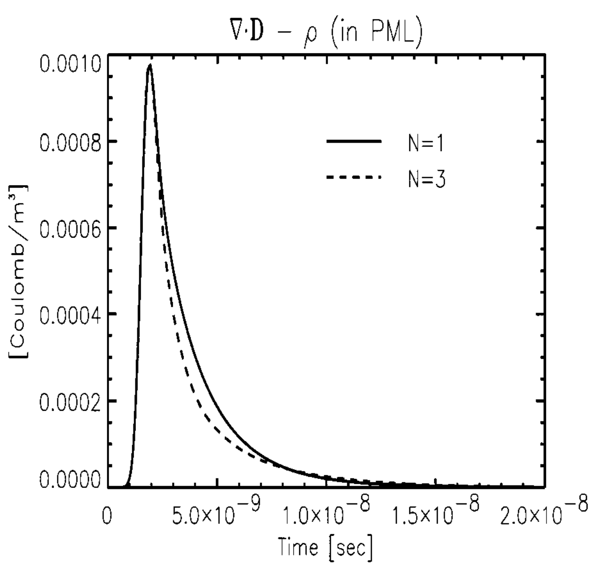

FIG. 3. Comparison of $\nabla \cdot \mathbf{D} - \rho$ in the PML region for one-dimensional, $N = 1$, and three-dimensional, $N = 3$, diffusion for the case $k = 0.1$.

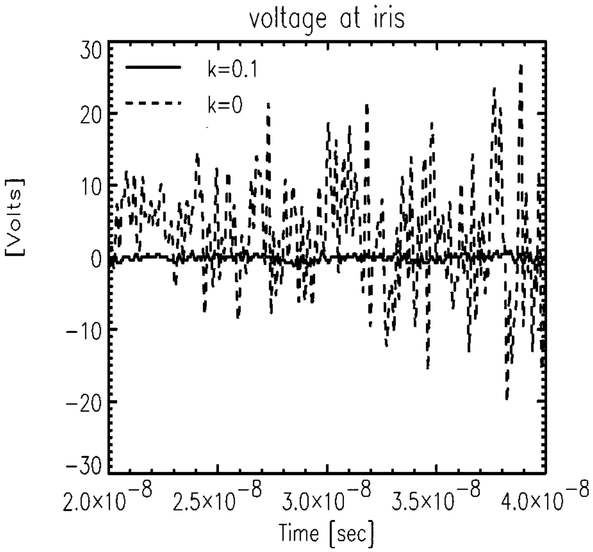

FIG. 4. Comparison of the voltage at the iris for the corrected $k = 0.1$, $N = 1$, and uncorrected $k = 0$ cases.

We can demonstrate some of the adverse effects of lack of charge conservation and the limitations of the correction by modifying our test problem slightly. First, we place the conducting walls at the same potential by short circuiting the input of the parallel-plate transmission line with a perfect electric conductor. Next, to amplify the errors in charge conservation we increase the beam current to 1 kA and switch from a Gaussian pulse to a 1 ns rise time ramp excitation. In Fig. 4 we compare the line integral of the electric field from the iris to the upper plate at the middle of the transmission line for $k = 0$ and $k = 0.1$. We expect a zero potential in steady state because of the short circuit. In Fig. 5, we compare

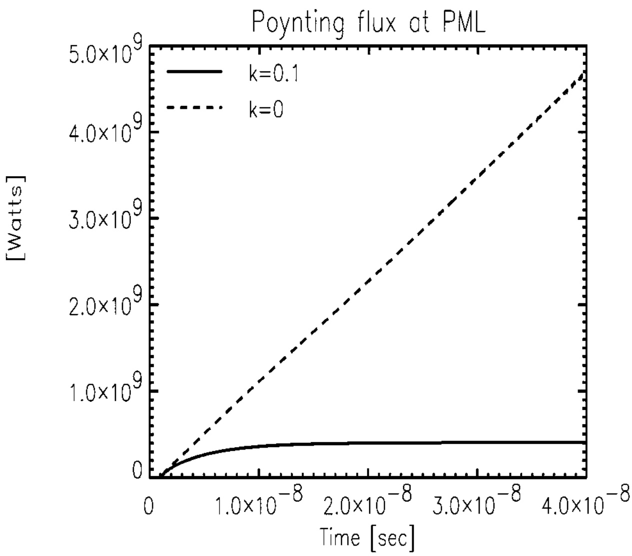

FIG. 5. Comparison of the Poynting flux at the PML interface for the corrected $k = 0.1$, $N = 1$, and uncorrected $k = 0$ cases.

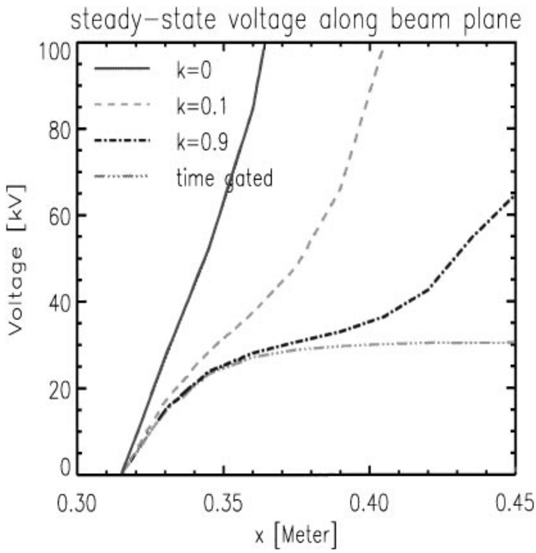

FIG. 6. Comparison of the steady-state voltage along the plane of the beam for uncorrected ($k = 0$), corrected ($k = 0.1$, $k = 0.9$), and time gated cases.

the Poynting flux through the PML interface for $k = 0$ and $k = 0.1$. Because the sheet beam is highly relativistic we can treat it as the third conductor in a triple conductor parallel-plate transmission line driven in a differential mode to estimate the voltage of the TEM wave driven by the beam current. Both this simple analytical analysis and numerical results from transit-time-isolated simulations predict a steady-state flux on the order of 30 MW; however, the observed flux is considerably larger. This worst case example of a large constant flux of charge through the boundary serves to demonstrate some of the limitations of the diffusive correction. The amount of diffusion is limited by several factors: the stability constraints on the diffusion constant and electromagnetic absorption requirements which determine the size of the diffusive PML region. In Fig. 6 we show the steady-state voltage (computed from a line integral of the electric field in the plane of the beam) as a function of position from the emission point to the PML interface for several different diffusion constants as well as results from a simulation where the effects of terminating the beam have been removed by transit-time isolation. We expect similar improvements as the size of the PML region is increased. Clearly the limitations on the diffusive correction do not allow the method to totally remove the buildup of charge and there is a resulting nonphysical power flow. For smaller initial beam velocities such charge buildup could slow down the particles in the beam. However, we must stress that this example was chosen to demonstrate the adverse effects when no corrections are made but does not fall into the regime of applications appropriate for the present method. Our practical application of this method has been limited to cases were the primary power flux through the boundary is due to electromagnetic field energy.

CONCLUSIONS

In this paper we have presented a modification to the Berenger PML absorbing boundary condition that allows it to be used in electromagnetic PIC simulations where the primary power flow through the boundary is due to electromagnetic radiation. It is our hope that the superior absorbing properties of the PML combined with this first-order correction for the treatment of particles will facilitate improved modeling of practical structures containing dispersive, multi-mode wave propagation and/or electromagnetic radiation in the presence of particles.

ACKNOWLEDGMENTS

The authors thank Dr. Stephen Rosenthal of Sandia National Laboratories for reviewing the original manuscript. The authors also thank the anonymous reviewers for their many constructive comments. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed–Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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