Maxwell Equation solver for plasma simulations based on mixed potential formulation

A. Hakim[*], U. Shumlak[†], C. Aberle[‡] & J. Loverich[§]
Aerospace and Energetics Research Program, University of Washington, Seattle, WA 98195-2600.

New algorithms for solving Maxwell's equations written in their mixed potential form are presented. Numerical solutions to Maxwell's equations are traditionally obtained using the finite difference time domain method, or the method of moments. Although these methods are successful in obtaining accurate solutions for problems on rectangular grids, they have inherent limitations when applied to non–orthogonal grids, specially of the type used in computational fluid dynamics applications. Two methods, the first based on finite volume schemes for hyperbolic conservation laws, and the second based on a finite difference scheme which gives a third order accurate spatial and second order accurate temporal algorithm are presented. Results to show that our algorithm perform well when compared to analytical solutions are shown. It is also shown that the algorithms handle the difficult case of absorbing boundary condition correctly.

Nomenclature

$\mathbf{E}$	Electric field, volts/m
$\mathbf{B}$	Magnetic flux density, weber/m^2
ρ_c	volume charge density, coulomb/m^2
$\mathbf{J}$	current density, amperes/m^2
ϵ_0	permittivity of free space, farad/m
μ_0	permeability of free space, henry/m
c	speed of light, m/s
ϕ	scalar potential, volts
$\mathbf{A}$	vector potential, weber/m

Introduction and motivation

Numerical solutions to Maxwell's equations are required in a number of fields, including, among others, geophysics, circuit analysis and design, radar detection of vehicles, electromagnetic wave propagation in tissue, and plasma physics. Among the most commonly used methods for solving Maxwell's equations are the finite difference time domain (FDTD) method and the method of moments (MOM).

FDTD[1] method is based on finite–differencing the Maxwell field equations in their differential form on a uniform rectangular grid. This method is used when the electromagnetic (EM) field quantities are required at all temporal and spatial points in the computational space and specially if the medium properties are continuous functions of space and/or of frequency. The drawbacks of the FDTD method is that it requires a staggered grid in both space and time to maintain second order accuracy and that it is difficult to handle complex geometries. The method of moments is based, on the other hand, on the solution of integral equations derived from the frequency domain Maxwell's equations. As is common with integral equation solution methods the MOM is based on Green's function for the problem. This reduces the EM problem to one of finding equivalent currents on the domain surfaces. The MOM[2] is applied mainly to circuit problems and those involving scattering of electromagnetic waves from complex geometries. For such configurations (for example, scattering from aircraft bodies) the MOM has a distinct advantage over the FDTD method: the MOM requires only surface meshes while FDTD requires a space mesh for complete domain. This leads to tremendous saving in both memory and execution time for codes implementing these methods. The disadvantage of the MOM is that it is a frequency domain method (although time domain MOM have been reported recently) and that it can not handle volume distributed sources well.

In this work a electromagnetic field solver based on the mixed potential formulation[3] of Maxwell's equations is described. The intended application of the solver is for a two-fluid plasma model,[4] which treats the plasma as a combination of an electron and ion fluids coupled through their electromagnetic fields. In this application the electromagnetic fields contribute source terms to the electron and ion fluid equations, while the electron and ion currents contribute source terms to the electromagnetic field equations. Our initial approach to solve Maxwell's equations was based on traditional computational fluid dynamic techniques (CFD) for hyperbolic conservation laws.[5] Although our solver works well in one dimension, in two dimensions large damping of the fields, which is especially severe for problems involving static discrete current

[*]AIAA member
[†]AIAA senior member
[‡]AIAA member
[§]AIAA member

sources, is observed. As a way to overcome this the Maxwell's equations can be recast in their mixed potential form. The advantage of this formulation is that it reduces Maxwell's equations to a set of inhomogeneous wave equations which can be solved using standard CFD techniques. A further advantage of this approach is that the resulting equations are uncoupled when formulated on rectangular grids which makes the solution technique much simpler.

The rest of the paper is organized as follows. First a brief derivation of the mixed potential equations from Maxwell's equations is presented. The implementation of boundary conditions is discussed, which can be difficult to handle properly on open, outflow boundaries. A number of these *absorbing boundary conditions* of which the method of using *perfectly matched layers* (PML) is described in some detail. Results with our algorithms and directions for future work are outlined.

Problem Formulation

Electromagnetic fields in homogeneous isotropic media are described by Maxwell's equations[3]

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \ , \tag{1}$$

$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J} \ , \tag{2}$$

$$\nabla \cdot \mathbf{E} = \frac{\rho_c}{\epsilon_0} \ , \tag{3}$$

$$\nabla \cdot \mathbf{B} = 0 \ , \tag{4}$$

where $\mathbf{E}$ is the electric field, $\mathbf{B}$ is the magnetic flux density, ρ_e is the charge density, $\mathbf{J}$ is the current density, and ϵ_0 and μ_0 are the permittivity and permeability of free space respectively. To rewrite these equations in the mixed potential formulation the scalar potential ϕ, and vector potential $\mathbf{A}$ are introduced by defining

$$\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t} \ , \tag{5}$$

$$\mathbf{B} = \nabla \times \mathbf{A} \ , \tag{6}$$

to obtain a set of inhomogeneous wave equations

$$\nabla^2 \phi - \mu_0 \epsilon_0 \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho_c}{\epsilon_0} \tag{7}$$

$$\nabla^2 \mathbf{A} - \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu_0 \mathbf{J} \ . \tag{8}$$

In obtaining these equations it is assumed that the potentials satisfy the Lorentz gauge condition

$$\nabla \cdot \mathbf{A} = -\mu_0 \epsilon_0 \frac{\partial \phi}{\partial t} \ , \tag{9}$$

In this paper results for two dimensional problems are presented, for which Eqs. (7) and (8) reduce, on rectangular cartesian grids, to

$$\frac{1}{c^2}\frac{\partial^2 f}{\partial t^2} - \frac{\partial^2 f}{\partial x^2} - \frac{\partial^2 f}{\partial y^2} = S \ , \tag{10}$$

where, $c^2 = (\mu_0 \epsilon_0)^{-1}$ and for $f \in \{\phi, A_x, A_y, A_z\}$, and $S \in \{\rho_c/\epsilon_0, \mu_0 J_x, \mu_0 J_y, \mu_0 J_z\}$. It is clear from this set of equations that for cartesian meshes an algorithm to solve the inhomogeneous wave equation needs to be developed, and then repeatedly used to solve for each variable f.

Algorithms

Two different algorithms to solve the inhomogeneous wave equations, Eqs. (7) and (8) or, on cartesian grids, Eq. (10), are explored. The first algorithm consists of rewriting the wave equation as a set of first order equations and then using standard finite volume high resolution schemes for hyperbolic equations to solve the resulting system. This approach is more general as it is based on the finite volume method and can thus take into account arbitrary grids. The second approach used is that of finite differencing the equations directly. Each of these methods is discussed briefly in the following subsections.

Finite Volume approach

To use methods developed for hyperbolic systems of equations, the wave operator in the governing equations are rewritten by defining,[5,6]

$$u = \frac{\partial f}{\partial t} \ , \tag{11}$$

$$\mathbf{v} = \nabla f \ , \tag{12}$$

to get a set of linear first order hyperbolic equations

$$\frac{1}{c^2}\frac{\partial u}{\partial t} - \nabla \cdot \mathbf{v} = S \tag{13}$$

$$\frac{\partial \mathbf{v}}{\partial t} - \nabla u = 0 \ . \tag{14}$$

This set of equations is solved using a high–resolution shock capturing scheme based on solutions of the Riemann problem. The source term is treated by using Strang–splitting,[5] which splits each time step advance into three sub–steps. The first step solves the source free problem over a half time-step, the second the flux free problem (but with sources) over a full time step, and the third again solves the source free problem over half a time step. At each step the values of the previous step are used as input data. Strang splitting ensures that that the method maintains second order accuracy in the presence of sources.

Finite Difference approach

To solve the inhomogeneous wave equations using finite differences on arbitrary grids the Laplacian operator is recalculated by applying a grid transformation from the physical space, (x, y), to the grid space, (ξ, η), using[7]

$$\nabla^2 f = \frac{1}{\sqrt{g}} \mathrm{div}_\xi \cdot \left(\sqrt{g} \mathcal{G}^{-1} \nabla_\xi f\right) \ , \tag{15}$$

where $\mathcal{G}$ is the metric tensor, $g = \det \mathcal{G}$, and div_ξ and ∇_ξ are the divergence and gradient operators in (ξ, η) space respectively. With this the transformed equations become

$$\frac{1}{c^2}\frac{\partial^2 f}{\partial t^2} - \frac{1}{\sqrt{g}}\text{div}_\xi \cdot \left(\sqrt{g}\mathcal{G}^{-1}\nabla_\xi f\right) = S \; . \tag{16}$$

To solve this equation a second order central difference approximation in time and a third order upwind biased difference approximation in space is used. The third order accuracy is achieved by using the difference approximations of the type

$$\frac{\partial^2 f}{\partial \xi^2} = \frac{f_A - 3f_B + 2f_{BB}}{\xi_A^2 - 3\xi_B^2 + \xi_{BB}^2} \; , \tag{17}$$

where A, B, BB are the downwind point and two upwind points respectively. The actual direction of differencing used at a node depends on the local direction of wave propagation at that node. This scheme, which is similar to the QUICK (Quadratic Upwind Interpolation of Convective Kinematics) scheme, ensures third order accuracy while enforcing proper upwinding.

Boundary conditions

The boundary condition for Maxwell's equations depend on the type of problem being solved. In general, in the absence of surface charges and surface currents, it is required that the tangential components of the electric field vector and magnetic field vector are continuous across boundaries. In addition, it is also required that normal components of the electric displacement vector and the magnetic flux density vector are continuous across boundaries. Thus,[3]

$$\mathbf{n} \times \mathbf{E}_- = \mathbf{n} \times \mathbf{E}_+ \; , \tag{18}$$

$$\mathbf{n} \times \mathbf{H}_- = \mathbf{n} \times \mathbf{H}_+ \; , \tag{19}$$

and

$$\mathbf{n} \cdot \mathbf{D}_- = \mathbf{n} \cdot \mathbf{D}_+ \; , \tag{20}$$

$$\mathbf{n} \cdot \mathbf{B}_- = \mathbf{n} \cdot \mathbf{B}_+ \; , \tag{21}$$

where the subscripts $+, -$ represent the exterior and the interior of the boundary respectively, $\mathbf{n}$ is a unit vector on the surface, and where, $\mathbf{D} = \epsilon_0 \mathbf{E}$ and $\mathbf{H} = 1/\mu_0 \mathbf{B}$. In general, it is straightforward to use these equations, along with the definitions Eqs. (5) and (6), to derive the corresponding boundary conditions for the potential equations.

The treatment of open boundaries, on the other hand, is difficult. To treat open boundaries properly the outgoing waves at the boundary must get "absorbed", or equivalently, not show any spurious oscillations. A number of methods can be used to enforce these absorbing boundary conditions (ABCs). One of the simplest methods is to split the wave operator into outgoing and ingoing wave equations (one way wave equations, or the advection equation) and then solve these split equations at the boundaries. For one dimensional problems this splitting can be done exactly, and hence all outgoing waves can be completely absorbed. Unfortunately, in higher dimensions such a splitting can only be done approximately. This approximate splitting causes a fraction of the outgoing waves to get reflected back into the domain, which potentially can cause large inaccuracies in the interior solution. Moore *et al.*[8] have studied various operator splitting methods and their effects on the interior solution in detail. In our code the so called second order Mur absorbing boundary conditions is implemented, which is based on splitting the two–dimensional wave operator to second order accuracy.

The second type of ABC explored is the Perfectly Matched Layer (PML) method.[9,10] The PML method essentially consists of adding a few layers of cells outside the domain in which modified equations are solved. These modified equations are constructed such that they admit non oscillating evanescent waves as solutions. This ensures that all incident waves decay as they propagate into the PML layer, thus preventing any spurious reflections. In our code a recently proposed optimal finite difference approximation of PML[11] which ensures that the reflection from the boundaries is minimum is implemented.

Results

To test our algorithms a number of simple problems for which analytical solutions are available were solved. In most cases it was seen that on rectangular grids both the finite volume method based on the Riemann solver, and the finite difference method based on the QUICK scheme give similar results. The results shown below are all obtained from the finite difference scheme. It was found, though, that the finite volume method does not perform well when solving problems with open boundaries and shows considerable spurious reflection. This problem arises due to the fact that on open boundaries the outgoing wave speeds were set to zero, which is equivalent to using the first order accurate splitting of the one–dimensional wave operator. Currently the use of PML layers in the finite volume algorithm is being explored.

The first test problem is that of wave propagation in a square wave guide $L = 20$ units to a side. For this problem a 100×100 grid was used with a sinusoidal initial condition $\phi(x, y, 0) = \sin(2\pi x/L)\sin(2\pi y/L)$ which is also an eigenfunction for the wave equation. Fig. (1) shows the calculated potential at time $t = 20$ while, Fig. (2) shows the potential $\phi(x, y = 5, t = 20)$. Comparison with analytical results for a square wave guides shows that the computed results have an RMS error of less than a percent.

The second test problem solved is that of evaluating

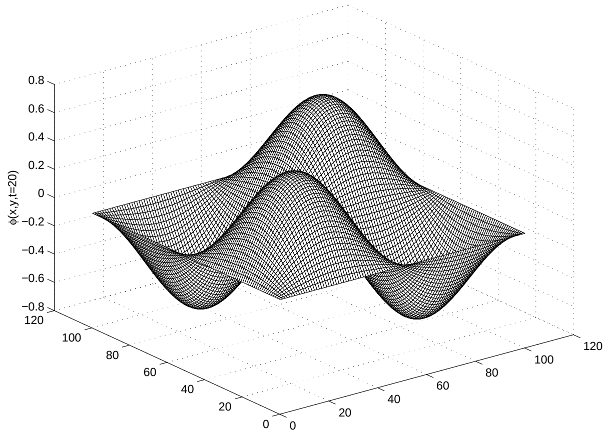


Fig. 1 Calculated solution to wave guide problem at $t = 20$. The wave guide is square and is initialized with a sinusoidal potential.

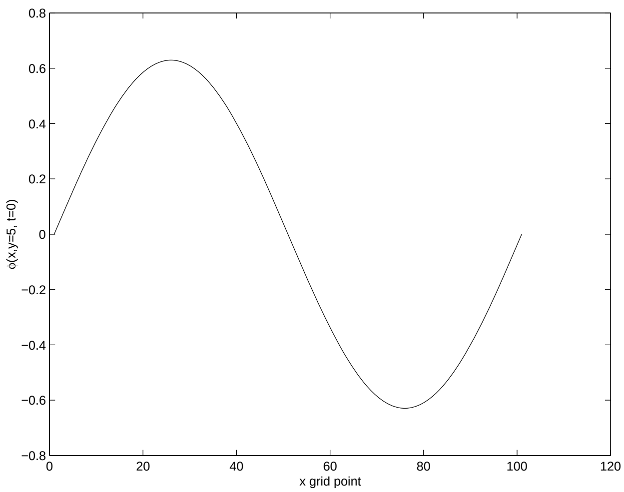


Fig. 2 Calculated solution to wave guide problem at $t = 20$. The plot shows the potential along a line parallel to the X–axis at $y = 5$.

the potential around a square current carrying conductor in an open domain. Fig. (3) shows the potential at time $t = 80$. From this figure it is seen that the potential has yet to reach a steady–state value. Fig. (4) shows the potential at time $t = 180$ at which the potential has reached a steady state value. Fig. (5) shows the magnetic field along the X–axis. When compared with the exact magnetic field obtained by using Ampere's law it is seen that the total RMS error is about 1.5%. It should be mentioned that this problem, although it seems simple, is a difficult one to solve numerically, specially using finite volume methods using approximate Riemann solvers. It is observed that when these methods are applied to the field equations directly the calculated fields are approximately zero everywhere except along the X and Y axis.

To tests the efficacy of the PML ABC a simulation with a plane wave moving through a rectangular domain was run. The results for this test are shown in

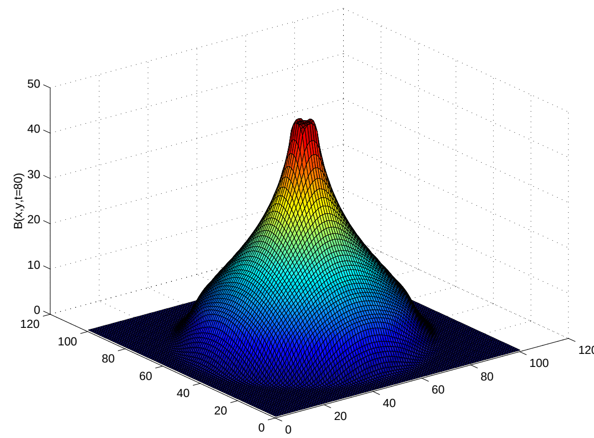


Fig. 3 Calculated magnetic field for a square current carrying conductor at time $t = 80$.

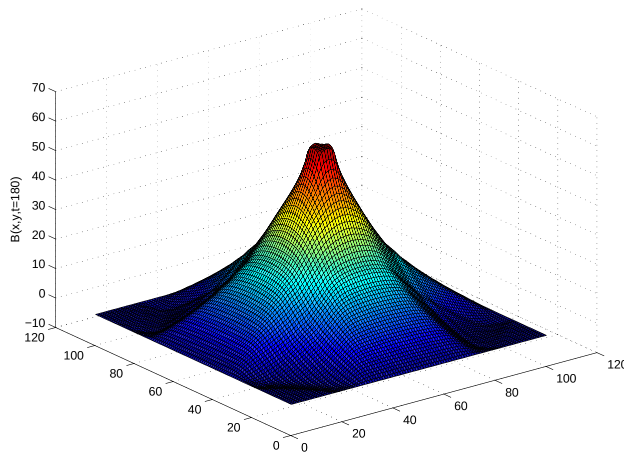


Fig. 4 Calculated magnetic field for a square current carrying conductor at time $t = 180$.

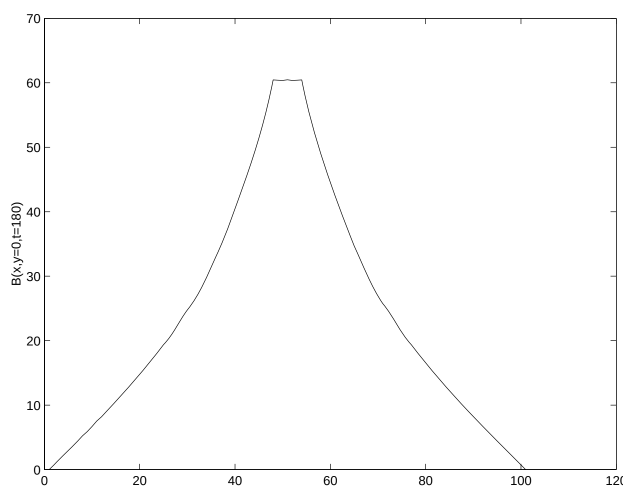


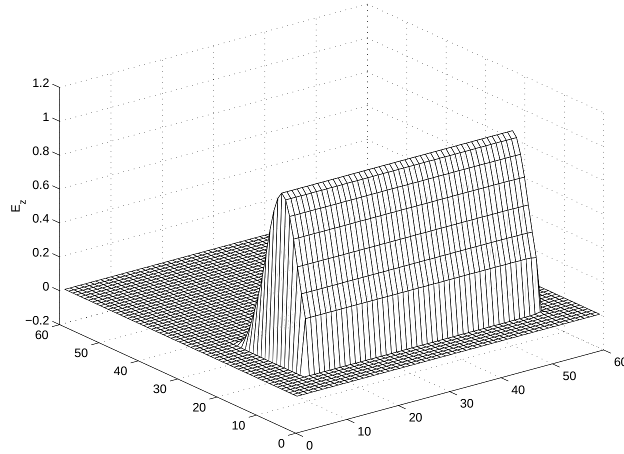
Fig. 5 Calculated magnetic field for a square current carrying conductor at time $t = 180$. This figure shows the magnetic field along the X–axis

Fig (6). From the snapshots of the electric field shown in this figure it is clear that the plane wave, on hitting the PML region, gets completely absorbed.

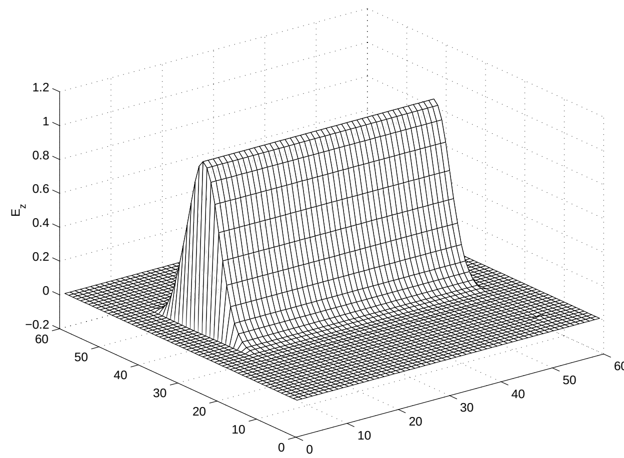
Conclusions and further work

In this paper two different algorithms for solving Maxwell's equations in their mixed potential formulation were presented. It was shown that the results obtained by these algorithms compare well with analytical solutions. It was also shown that the difficult case of open boundary conditions was handled correctly.

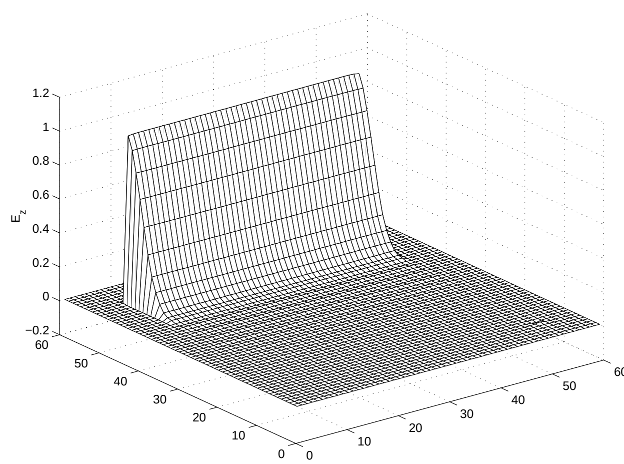
As an extension to the work presented here the PML boundary conditions are being implemented for the for the finite volume algorithm. Further, work is being done to integrate the electromagnetic solvers developed here into the fluid solver to study plasma physics.



a) $t = 40$



b) $t = 80$



c) $t = 120$

Fig. 6 Propagation of a plane wave through a rectangular domain. The plane wave hits the far wall and gets absorbed in the PML region. For this run 8 PML layers were used.

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