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Short Note

Boundary conditions for Maxwell solvers

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1. Introduction

We consider the properties of numerical solutions of a wave equation for the electric field **E**, [3],

$$\left(\frac{c\Delta t}{2}\right)^2 \nabla\times\nabla\times\mathbf{E} + \mathscr{K}\cdot\mathbf{E} = \mathbf{S}, \tag{1}$$

which arises in implicit plasma simulations and is similar to those that occur in many contexts. Compared with the standard Helmholtz equation [6, p. 68], $(c\Delta t/2)^2$ replaces $-(c/\omega)^2$, and Eq. (1) is solved each time step (instead of for each value of ω) for **E** with **S** given. The source term, **S**, is neither divergence nor curl-free in general.

Specifically, we ask under what conditions charge conservation is satisfied. Namely, do numerical solutions of Eq. (1) satisfy Poisson's equation,

$$\nabla\cdot[\mathscr{K}\cdot\mathbf{E} - \mathbf{S}] = 0, \tag{2}$$

which is derived from Eq. (1) by forming its divergence. We note that the dielectric susceptibility, $\mathscr{K}$, is a tensor with symmetric and anti-symmetric components.

A number of reasons why the numerical solutions may not satisfy Eq. (2) are given in Jiang et al. [7]. Among them are parasitic modes and errors in the difference equations that cause them not to satisfy the vector identity,

$$\nabla\cdot\nabla\times\nabla\times\mathbf{E} = 0. \tag{3}$$

In addition they cite a more fundamental reason: The Maxwell equations comprise eight equations with only six unknowns so that solutions are overdetermined. Their remedy is the addition of unknowns to the equations, whose presence contributes nothing to the solutions of Eq. (1), except additional boundary conditions that assure a solution of Eq. (2). Here we assume that neither of the first two errors occurs in the numerical solutions, and limit our consideration to a third source of error; inconsistently formulated boundary conditions. Our approach is to examine a weak formulation of Eq. (1) that displays explicitly the boundary conditions for which a solution of Eq. (1) also satisfies Eq. (2).

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2. The weak formulation

We integrate the scalar product of Eq. (1) with an arbitrary but sufficiently smooth test function $\mathbf{E}' \in R^3$, over the domain $D \in \mathscr{R}^3$,

$$\mathscr{I} = \int_D \mathbf{E}' \cdot \left[\left(\frac{c\Delta t}{2} \right)^2 \nabla \times \nabla \times \mathbf{E} + \mathscr{K} \cdot \mathbf{E} - \mathbf{S} \right] \mathrm{d}V. \tag{4}$$

We further require that $\mathbf{E}'$ and $\mathbf{E}$ satisfy the same boundary conditions. Any $\mathbf{E}$ that solves Eq. (1) yields $\mathscr{I} = 0$.

We note there exists for $\mathbf{E}$ a (standard) Helmholtz decomposition,

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \tag{5}$$

where $\nabla \times \nabla\phi = 0$ and $\nabla \cdot \mathbf{A} = 0$. When either $\hat{\mathbf{n}} \cdot \mathbf{A} = 0$, or $\phi = \text{const}$ on ∂D, the vector and scalar potentials are orthogonal,

$$\int_D \mathbf{A} \cdot \nabla\phi \mathrm{d}V = 0. \tag{6}$$

We replace $\mathbf{E}'$ in Eq. (4) with its Helmholtz decomposition. There results two integrals, $\mathscr{I} = \mathscr{I}_\mathbf{A} + \mathscr{I}_\phi$. $\mathscr{I}_\phi$, for example is given by,

$$\mathscr{I}_\phi = \int_D -\nabla\phi' \cdot \left[\left(\frac{c\Delta t}{2} \right)^2 \nabla \times \nabla \times \mathbf{E} + \mathscr{K} \cdot \mathbf{E} - \mathbf{S} \right] \mathrm{d}V. \tag{7}$$

Since $\nabla\phi'$ or $\mathbf{A}'$ are themselves suitable test functions when $\mathbf{E}'$ is, $\mathscr{I}_\mathbf{A} = \mathscr{I}_\phi = 0$.

Noting that $-\nabla\phi' \cdot [\nabla \times \nabla \times \mathbf{E}] = \nabla \cdot [\nabla\phi' \times \nabla \times \mathbf{E}]$ by Poynting's theorem, we integrate Eq. (7) by parts to derive $\mathscr{I}_\phi = \mathscr{I}_{\mathscr{V}\phi} + \mathscr{I}_{\mathscr{S}\phi}$, where $\mathscr{I}_{\mathscr{V}\phi}$ is,

$$\mathscr{I}_{\mathscr{V}\phi} = \int_D \phi' \nabla \cdot [\mathscr{K} \cdot \mathbf{E} - \mathbf{S}] \mathrm{d}V, \tag{8}$$

and $\mathscr{I}_{\mathscr{S}\phi}$ is,

$$\mathscr{I}_{\mathscr{S}\phi} = \int_{\partial D} \hat{\mathbf{n}} \cdot [(\nabla\phi' \times \nabla \times \mathbf{E})] - \hat{\mathbf{n}} \cdot [\mathscr{K} \cdot \mathbf{E} - \mathbf{S}]\phi' \, \mathrm{d}S. \tag{9}$$

We can now state the following theorem:

Theorem 1. *Iff* $\mathscr{I}_{\mathscr{S}\phi} = 0$, *any* $\mathbf{E}$ *that satisfies Eq.* (1) *also satisfies Poisson's equation*, *Eq.* (2).

Proof. If $\mathscr{I}_{\mathscr{S}\phi} = 0$, then by Eq. (7), $\mathscr{I}_{\mathscr{V}\phi} = 0$ for any suitable ϕ'. Therefore the integrand is zero everywhere in D and Poisson's equation, Eq. (2), is satisfied.

If $\mathscr{I}_{\mathscr{S}\phi} \neq 0$, then by Eq. (7), $\mathscr{I}_{\mathscr{V}\phi} = -\mathscr{I}_{\mathscr{S}\phi}$, the integrand cannot be zero everywhere and Eq. (2) is not satisfied.

Consider $\mathscr{I}_{\mathscr{S}\phi}$. It must be zero for any suitable ϕ', including ϕ corresponding to the Helmholtz decomposition of the solution to (1), $\mathbf{E}$.

The first term in the integrand in Eq. (9) will be zero if either ∂D is a conductor with $\phi' = \text{const}$ on ∂D,

$$(\hat{\mathbf{n}} \times \nabla\phi') = 0, \tag{10}$$

or ∂D is a magnetic symmetry boundary with $\hat{\mathbf{n}} \times \mathbf{B} = \text{const}$ on ∂D so that

$$(\hat{\mathbf{n}} \times \nabla \times \mathbf{E}) = 0. \tag{11}$$

The second term in Eq. (9) will be zero for a conductor with $\phi' = \text{const}$ on ∂D if a compatibility condition is satisfied,

$$\int_{\partial D} \hat{\mathbf{n}} \cdot [\mathscr{K} \cdot \mathbf{E} - \mathbf{S}] \mathrm{d}S = 0. \tag{12}$$

If, as for a magnetic symmetry surface, ϕ' varies on ∂D, then the integrand in Eq. (9) is zero if and only if a local charge conservation condition is satisfied by the solution everywhere on ∂D,

$$\hat{\mathbf{n}} \cdot [\mathscr{K} \cdot \mathbf{E} - \mathbf{S}] = 0. \qquad \square \tag{13}$$

3. Uniqueness

We compare the boundary conditions, Eqs. (10)–(13) with those derived by integrating Eq. (4) by parts. We assume, as above, that $\mathbf{E}$ is a solution of Eq. (1) so that $\mathscr{I} = 0$. A surface and a volume contribution comprise $\mathscr{I}$. The surface contribution,

$$\mathscr{I}_{\mathscr{S}} = \int_{\partial D} -\hat{\mathbf{n}} \cdot [(\nabla \times \mathbf{E}) \times \mathbf{E}'] \mathrm{d}S, \tag{14}$$

is zero if $\hat{\mathbf{n}} \times \mathbf{E}' = 0$, corresponding to a conductor, Eq. (10), or if $\hat{\mathbf{n}} \times \nabla \times \mathbf{E} = 0$, corresponding to a magnetic symmetry surface, Eq. (11). There are no conditions like Eqs. (12) and (13) to be inferred from $\mathscr{I}_{\mathscr{S}}$.

We now consider the volume contribution, $\mathscr{I}_{\mathscr{V}}$,

$$0 = \int_D \left(\frac{c\Delta t}{2}\right)^2 \nabla \times \mathbf{E} \cdot \nabla \times \mathbf{E}' + \mathbf{E}' \cdot (\mathscr{K} \cdot \mathbf{E} - \mathbf{S}) \mathrm{d}V. \tag{15}$$

With a standard form of the susceptibility, the electric field energy, $\mathbf{E} \cdot \mathscr{K} \cdot \mathbf{E}$ is positive for any non-zero field,

$$\mathbf{E} \cdot \mathscr{K} \cdot \mathbf{E} = (1 + \epsilon_P)\mathbf{E}^2 + \epsilon_{\mathrm{H}} \mathbf{E} \cdot \mathbf{E} \times \mathbf{B} + \epsilon_{\parallel} (\mathbf{E} \cdot \mathbf{B})^2, \tag{16}$$

where $\epsilon_{\mathbf{P}}$, ϵ_{H}, and $\epsilon_{\parallel}$ are the Pederson, Hall and parallel dielectric permeabilities (or conductivities in the case of a collisional plasma). The field energy term is clearly a quadratic form, because the anti-symmetric term cancels.

Let us suppose that $\mathbf{E}_1$ and $\mathbf{E}_2$ are both solutions of the variational problem with either conducting wall or magnetic symmetry boundary conditions, Eq. (4), so that $\mathscr{I}(\mathbf{E}_1) - \mathscr{I}(\mathbf{E}_2) = 0$. With $\mathbf{E}' = \mathbf{E}_1 - \mathbf{E}_2$,

$$0 = \int_D (c\theta\Delta t)^2 \nabla \times \mathbf{E}' \cdot \nabla \times \mathbf{E}' + (1 + \epsilon_{\mathrm{P}})\mathbf{E}' \cdot \mathbf{E}' + \epsilon_{\parallel} (\mathbf{E}' \cdot \mathbf{B})^2 \, \mathrm{d}V. \tag{17}$$

Since every term in Eq. (17) is positive for any non-zero value of $\mathbf{E}$, the equation can be satisfied only by $\mathbf{E}' = \mathbf{E}_1 - \mathbf{E}_2 = 0$, proving that the solution to the variational problem uniquely minimizes $\mathscr{I}$.

Moreover, Theorem 1 shows that Eq. (2) is satisfied because $\mathscr{I}_{\mathscr{S}\phi} = 0$ with boundary conditions given by Eq. (12) or (13). Therefore, a unique solution of Eq. (1) is obtained that also satisfies Poisson's equation, Eq. (2), if one applies the boundary conditions,

$$\hat{\mathbf{n}} \times \mathbf{E} = 0, \quad \int_{\partial D} \hat{\mathbf{n}} \cdot (\mathscr{K} \cdot \mathbf{E} - \mathbf{S}) \mathrm{d}S = 0, \tag{18}$$

for a conducting wall, and

$$\hat{\mathbf{n}} \times \nabla \times \mathbf{E} = 0, \quad \hat{\mathbf{n}} \cdot (\mathscr{K} \cdot \mathbf{E} - \mathbf{S}) = 0, \tag{19}$$

for a magnetic symmetry boundary.

4. Numerical tests

We include numerical test results of the boundary conditions, Eqs. (18) and (19) with an implicit plasma simulation code, CELESTE. It solves a finite difference approximation to Eq. (1) using a matrix-free, Krylov solver with periodic boundary conditions in x and y, and specified boundary conditions in z. Details of the implicit formulation are given in [10]. The finite difference approximation is given in detail in [2]. As noted in [10], the difference approximations satisfy Eq. (3) only on a uniform, rectilinear grid. However, there are methods which also satisfy Eq. (3) on non-uniform grids [5].

Our test case is a calculation of the lower-hybrid-drift instability, which is described in detail in [4]. The uniform, rectilinear grid comprises 64 cells in y and in z, and one cell in x. The time step is $\omega_{\text{pi}}\Delta t = 0.5$, where ω_{pi} is the ion plasma frequency, and the ion/electron mass ratio is, $m_{\text{i}}/\text{m}_{\text{e}} = 180$. There are 220,000 particles in the simulation, or 27 electrons and 27 ions per cell initially. Random fluctuations in the number of particles cause as much as a ≈20% cell to cell variation in the magnitude of the conductivity $\mathbf{K}$ in Eq. (1).

4.1. Case 1

In Case 1, the magnetic field is tangent to the top and bottom boundaries and particles are reflected in the conducting case, Table 1. We vary the tolerance for the solver over 12 orders of magnitude in the solution of Eq. (1) and show that Poisson's equation, Eq. (2), converges as Eq. (1) converges. Table 1 for conducting boundaries, Eq. (18), and Table 2 for magnetic symmetry boundaries, Eq. (19), summarize the results.

The error measures are the ratio of the L_2 norm of the residual error to the L_2 norm of the source, $\mathbf{S}$. Eq. (1), and the same ratio for the divergence of the residual and $\nabla \cdot \mathbf{S}$ for Poisson's equation, Eq. (2). (The contribution of errors in satisfying Eq. (3) are $\approx 10^{-18}$, which is small compared with even the smallest residual errors.) The number of iterations listed times 10 is the number of GMRES iterations to convergence. The ratio of the error in the solution of Eq. (2) to the error in Eq. (1) is never more than 2.

4.2. Case 2

For the magnetic symmetry boundary, Case 2, the magnetic field is perpendicular to the top and bottom boundaries, and simulation particles are absorbed there. In this case, a significant imbalance of charge builds, as the electrons are lost more rapidly than the ions.

The results for two convergence criteria are listed in Table 2. For Case 2a, convergence is measured by $\|\mathbf{F}\|_2$, the norm of the error in the solution of Eq. (1). For Case 2b, convergence is measured by the error in the solution of Eq. (2). The number of iterations for Case 2b is sometimes higher, but not always. At convergence, the ratio of the errors for Eqs. (1) and (2) for Cases 2a and 2b are comparable.

Table 1
In a calculation of the lower-hybrid-drift instability with electrically conducting boundaries, the errors in the wave equation and Poisson's equation decrease as the solver error tolerance decreases

Tolerance	Case 1 iterations	$\|\mathbf{F}\|_2$	$\|\nabla\cdot\mathbf{F}\|_2$
10^{-3}	2	7.2×10^{-4}	9.5×10^{-4}
10^{-5}	3	9.7×10^{-6}	9.1×10^{-6}
10^{-7}	5	9.8×10^{-8}	2.0×10^{-7}
10^{-9}	6	8.8×10^{-10}	1.5×10^{-9}
10^{-11}	8	9.3×10^{-12}	1.3×10^{-11}
10^{-13}	9	7.2×10^{-14}	1.2×10^{-13}
10^{-15}	11	7.7×10^{-16}	1.4×10^{-15}

Table 2
With magnetic symmetry boundary conditions, the solution error decreases as the error tolerance decreases

Tolerance	Case 2a iterations	$\|\mathbf{F}\|_2$	$\|\nabla\cdot\mathbf{F}\|_2$	Case 2b iterations	$\|\mathbf{F}\|_2$	$\|\nabla\cdot\mathbf{F}\|_2$
10^{-3}	2	7.3×10^{-4}	6.8×10^{-4}	2	7.3×10^{-4}	6.5×10^{-4}
10^{-5}	3	6.5×10^{-6}	1.0×10^{-6}	4	5.1×10^{-6}	9.3×10^{-6}
10^{-7}	4	9.8×10^{-8}	1.0×10^{-7}	4	9.8×10^{-8}	1.0×10^{-7}
10^{-9}	6	9.7×10^{-10}	2.2×10^{-9}	18	3.7×10^{-10}	9.4×10^{-10}
10^{-11}	7	7.9×10^{-12}	1.6×10^{-11}	14	4.0×10^{-12}	9.8×10^{-12}
10^{-13}	9	7.8×10^{-14}	1.3×10^{-13}	13	4.7×10^{-14}	9.6×10^{-14}
10^{-15}	10	8.4×10^{-16}	1.6×10^{-15}	17	4.2×10^{-16}	9.4×10^{-16}

The results are the same whether the error in the wave equation, Case 2a, or Poisson's equation, Case 2b, measures convergence.

5. Comments

We have shown analytically that correctly applied boundary conditions for a semi-discrete approximation to electromagnetic wave propagation in a plasma, Eq. (1), yield solutions that satisfy Poisson's equation, Eq. (2), and that these solutions are unique. Our numerical tests using a difference method that satisfies the vector identity, Eq. (3) and does not have parasitic modes yield results that are consistent with the analysis. We believe these results support the view that the spurious solutions discussed in [7] are the result of numerical error rather than a property of Maxwell's equations. We note, that the boundary conditions used in a previous paper [3], which were based on work described in [7], also yield accurate solutions for Eq. (1). However, the boundary conditions are more complex than Eqs. (18) or (19).

Generally speaking, Maxwell solvers that resolve electromagnetic waves solve initial value problems. For time resolution of electromagnetic waves, it is more efficient to march explicit equations than to solve systems of equations iteratively each time step. Of course, charge must be conserved, but it is dealt with within a hyperbolic framework by adding corrections [8], constraints [11], or, as in the case of the *div − curl* method, by satisfying the charge conservation equation on the boundary [7].

It may be interesting to consider embedding the solution of equations like Eq. (2), which occur in many contexts, in a wave equation. For example, one algorithm for ionospheric current flow solves Eq. (2) for a scalar potential field with a conductivity tensor in which the parallel conductivity is so high that $\mathbf{E} \cdot \mathbf{B} = 0$. This symmetry is exploited to obtain solutions in three dimensions by solving Eq. (2) in two dimensions with respect to a locally defined coordinate system [9]. However, to include inductive electric fields as well as scalar potential fields, one can solve Eq. (1) with appropriate values for the conductivity, $\mathbf{K}$. Similarly, subterranean water flow is modeled by solving d'Arcy's law with an anisotropic but symmetric permeability tensor [1]. The solutions are obtained in a local coordinate system in which the tensor is diagonalized. The advantage of embedding in these cases is that one replaces an elliptic operator with rough coefficients by one with constant coefficients.

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