1. Introduction

We consider the properties of numerical solutions of a wave equation for the electric field $E$, [2],

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

(1)

which is solved in implicit plasma simulations. Compared with the standard Helmholtz equation [4, p68], $(c\Delta t/2)^2$ replaces $-(c/\omega)^2$, and Eq. 1 is solved each time step (instead of for each value of $\omega$) 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,

$$
\nabla \cdot [K \cdot E - S] = 0,
$$

(2)

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

There are a number of reasons why the numerical solutions may not preserve charge conservation. There may be errors in the computation of the charge continuity equation, or the difference equations may not satisfy the vector identity,

$$
\nabla \cdot \nabla \times \nabla \times E = 0.
$$

(3)

Here we assume that neither of these 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.

2. The Weak Formulation

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

Boundary Conditions for Maxwell Solvers

J. U. Brackbill

ParticleSolutions, Portland, OR
\[ I = \int_D \mathbf{E}' \cdot \left[ \left( \frac{c \Delta t}{2} \right)^2 \nabla \times \nabla \times \mathbf{E} + \mathbf{K} \cdot \mathbf{E} - \mathbf{S} \right] dV. \] (4)

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

We note there exists for \( \mathbf{E} \) a (standard) Helmholtz decomposition,
\[ \mathbf{E} = -\nabla \phi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}, \] (5)
where \( \nabla \times \nabla \phi = 0 \) and \( \nabla \cdot \mathbf{A} = 0 \). When either \( \hat{n} \cdot \mathbf{A} = 0 \), or \( \phi = \text{const} \) on \( \partial D \), the vector and scalar potentials are orthogonal,
\[ \int_D \mathbf{A} \cdot \nabla \phi dV = 0. \] (6)

We replace \( \mathbf{E}' \) in Eq. 4 with its Helmholtz decomposition. There results two integrals, \( I = I_A + I_\phi \), for example is given by,
\[ I_\phi = \int_D -\nabla \phi' \cdot \left[ \left( \frac{c \Delta t}{2} \right)^2 \nabla \times \nabla \times \mathbf{E} + \mathbf{K} \cdot \mathbf{E} - \mathbf{S} \right] dV. \] (7)

Since \( \nabla \phi' \) or \( \mathbf{A}' \) are themselves suitable test functions when \( \mathbf{E}' \) is, \( I_A = I_\phi = 0 \).

Integrating Eq. 7 by parts yields \( I_\phi = I_{V\phi} + I_{S\phi} \), where \( I_{V\phi} \) is,
\[ I_{V\phi} = \int_D -\phi' \nabla \cdot [\mathbf{K} \cdot \mathbf{E} - \mathbf{S}] dV \] (8)
and \( I_{S\phi} \) is,
\[ I_{S\phi} = \int_{\partial D} \hat{n} \cdot [\nabla \times \mathbf{E} \times \nabla \phi'] - \hat{n} \cdot [\mathbf{K} \cdot \mathbf{E} - \mathbf{S}] \phi' dS. \] (9)

We can now state the following theorem;

**Theorem 1** If \( I_{S\phi} = 0 \), any \( \mathbf{E} \) that satisfies Eq. 1 also satisfies Poisson’s equation, Eq. 2.

Proof:

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

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

Consider \( I_{S\phi} \). It must be zero for any suitable \( \phi' \), including \( \phi \) 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 \( \partial D \) is a conductor with \( \phi' = \text{const} \) on \( \partial D \),
\[ (\hat{n} \times \nabla \phi') = 0, \] (10)
or \( \partial D \) is a magnetic symmetry boundary with \( \hat{n} \times \mathbf{B} = \text{const} \) on \( \partial D \) so that
\[ (\hat{n} \times \nabla \times \mathbf{E}) = 0. \] (11)
The second term in Eq. 9 will be zero for a conductor with \( \phi' = \text{const} \) on \( \partial D \) if a compatibility condition is satisfied,

\[
\int_{\partial D} \hat{n} \cdot [K \cdot E - S] \, dV = 0.
\]  

(12)

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

\[
\hat{n} \cdot [K \cdot E - S] = 0.
\]  

(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 \( E \) is a solution of Eq. 1 so that \( I = 0 \). A surface and a volume contribution comprise \( I \). The surface contribution,

\[
I_S = \int_{\partial D} \hat{n} \cdot [(\nabla \times E) \times E'] \, dS.
\]  

(14)

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

We now consider the volume contribution, \( I_V \),

\[
0 = \int_D (\frac{c \theta \Delta t}{2})^2 \nabla \times E' \cdot \nabla \times E' + (1 + \epsilon_P) E' \cdot E' + \epsilon_H (E \cdot B)^2 \, dV.
\]  

(15)

With a standard form of the susceptibility, the electric field energy, \( E \cdot K \cdot E \) is positive for any non-zero field,

\[
E \cdot K \cdot E = (1 + \epsilon_P) E^2 + \epsilon_H E \cdot E \times B + \epsilon_{\parallel} (E \cdot B)^2,
\]  

(16)

where \( \epsilon_P, \epsilon_H, \) 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 \( E_1 \) and \( E_2 \) are both solutions of the variational problem with either conducting wall or magnetic symmetry boundary conditions, Eq. 4, so that \( I(E_1) - I(E_2) = 0 \). With \( E' = E_1 - E_2 \),

\[
0 = \int_D (c \theta \Delta t)^2 \nabla \times E' \cdot \nabla \times E' + (1 + \epsilon_P) E' \cdot E' + \epsilon_{\parallel} (E' \cdot B)^2 \, dV.
\]  

(17)

Since every term in Eq. 17 is positive for any non-zero value of \( E \), the equation can be satisfied only by \( E' = E_1 - E_2 = 0 \), proving that the solution to the variational problem uniquely minimizes \( I \).

Moreover, Theorem 1 shows that Eq. 2 is satisfied because \( I_{S\phi} = 0 \) 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,
\[ \hat{n} \times \mathbf{E} = 0, \quad \int_{\partial D} \hat{n} \cdot (\mathbf{K} \cdot \mathbf{E} - \mathbf{S}) \, dS = 0, \quad (18) \]

for a conducting wall, and

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

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, Newton-Krylov solver with periodic boundary conditions in \( x \) and \( y \), and specified boundary conditions in \( z \). (We use a nonlinear solver for this linear problem simply for convenience.)

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 simulations use a \( 64 \times 64 \) zone grid in two dimensions with 220000 simulation particles.

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. The physical problem is described in [8].

The error measures are the ratio of the \( L_2 \) norm of the residual error to the \( L_2 \) norm of the source, \( \mathbf{S} \) in the solution of Eq. 1, and the same ratio for the divergence of the residual and \( \nabla \cdot \mathbf{S} \) for Poisson’s equation, Eq. 2. The number of Newton iterations is listed. For each of these there are up to 10 GMRES iterations. The ratio of the error in the solution of Eq. 2 to the error in Eq. 1 is never more than 2.

Table 1

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

5. Comments

We have shown that correctly applied boundary conditions for the wave equation, Eq. 1 yield solutions that satisfy Poisson’s equation, Eq. 2. An earlier paper [2], which was based on work described in [5], described more complex boundary conditions with a similar outcome. Compared with the present results, the accuracy of the earlier solutions is limited by the truncation error of the difference equations one solves on the boundary, and the coding is more complex. However, compared with the alternative, which is a separate solution of Poisson’s equation, Eq. 2, both are simpler. The variation in $\mathbf{K}$ from cell to cell and time step to time step makes solving Eq. 2 a classical rough coefficient problem. Our most successful attempt, using a multigrid preconditioner and a Newton-Krylov solver [3], never evolved from 2 dimensions to 3 or migrated to new computing platforms. By contrast, the number of iterations without preconditioner with a Newton-Krylov solver when applied to Eq. 1 is relatively low. One colleague remarked that in solving Eq. 1 for low frequency, electromagnetic plasma simulations seems to require only making a small correction to Ohm’s law with $\nabla \times \nabla \times \mathbf{E}$.

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 [6], constraints [9], or, as in the case of the \( \text{div} - \text{curl} \) method, by satisfying the charge conservation equation on the boundary [5].

However, 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, ionospheric current flow solves Eq. 2 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 [7]. 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.

Acknowledgements

This material is based upon work supported by the National Science Foundation under Grant No. 0614006. Many useful discussions with Giovanni Lapenta and Paolo Ricci are gratefully acknowledged.

References