DERIVATION OF A FINITE ELEMENT FORMULATION FROM A LAGRANGIAN FOR THE ELECTROMAGNETIC POTENTIALS

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Abstract

Conventional electromagnetic finite element solvers typically solve a weak formulation of the Helmholtz wave equation. While mathematically this approach is correct, it does not fully reflect the fundamental physics involved. We offer an alternative variational formulation which is not derived from the Helmholtz wave equation but is more fundamentally tied to the physics of the system: a Lagrangian for the electromagnetic potentials. Solving for the potentials directly allows for a natural accounting of the beam wave interaction through the interaction terms $\rho\phi$ and $\vec{A}\cdot\vec{J}$. It could also potentially avoid the issue of deleterious spurious modes inherent when selecting the Coulomb gauge and enforcing the subsequent divergence free condition, eliminating the need for vector basis functions. Herein we present the theory and the resulting formulation including a discussion on gauge fixing. We conclude with some numerical results demonstrating the potential of this formulation.

INTRODUCTION AND MOTIVATION

The finite element method (FEM) is a numerical method used to solve boundary value problems of partial differential equations. It does this by discretizing the solution space and approximating the partial differential equations by a set of ordinary differential equations, or in steady state, linear equations, on each element. This requires a variational or weak formulation of the problem such that the minimized function over the discretized space corresponds to the solution to the original problem.

Electromagnetic solvers typically solve a weak formulation of the Helmholtz wave equation, given by Eq. (1) and (2) in the source free case. Note that these equations are written in terms of the $\vec{E}$ and $\vec{B}$ fields, which are decoupled from each other. In magnetostatics and magnetodynamics, a magnetic vector or scalar potential is frequently used instead of solving for $\vec{B}$ directly.

$$(\nabla^2 + k^2)\vec{E} = 0 \tag{1}$$

$$(\nabla^2 + k^2)\vec{B} = 0 \tag{2}$$

An alternative approach we present here is to start with the Lagrangian for the electromagnetic potentials, ϕ, $\vec{A}$. This variational formulation results in Maxwell's equations when varied, naturally lending itself to finite element analysis (FEA). Furthermore, unlike weak forms derived explicitly from Maxwell's equations, the Lagrangian formulation is derived from and thus reflects the physics on a fundamental level, from the inherent symmetries to the beam-wave interaction.

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In this paper we will present a Lagrangian for use in electromagnetic FEA, demonstrating that it encodes Maxwell's equations and can account for arbitrary boundary conditions on the fields. We will then discuss the question of gauge fixing and spurious modes. We will demonstrate how we can avoid spurious modes, an issue which plagues numerical solvers of the Helmholtz equation, without needing to resort to vector basis functions. Finally, we conclude with a brief outline of the implementation of this formulation in C++ and plans for future work.

A LAGRANGIAN APPROACH

The classical Lagrangian for the electromagnetic four potential (separated into the electrostatic potential, ϕ and the magnetic vector potential, $\vec{A}$) is given by Eq. (3). Here ρ is the charge density and $\vec{J}$ is the current density.

$$\mathcal{L} = \int\int \frac{\epsilon}{2}\left(|\nabla\phi + \frac{\partial\vec{A}}{\partial t}|^2 - c^2|\nabla\times\vec{A}|^2\right) - \rho\phi + \vec{A}\cdot\vec{J}\,dv\,dt \tag{3}$$

It is worth noting that we could have used a Lagrangian written in terms of the electromagnetic fields, however working with the four-potential offers a natural accounting of beam-wave interactions through the $\rho\phi$ and $\vec{A}\cdot\vec{J}$ terms.

This Lagrangian can be shown to produce Maxwell's equations with magnetic wall boundary conditions when varied. To account for arbitrary boundary conditions, we add the term in Eq. (4).

$$\mathcal{L}_{\mathrm{BC}} = \int\int \frac{1}{i\omega}(-\nabla\phi - \frac{\partial\vec{A}}{\partial t})\cdot Y\cdot(-\nabla\phi^* - \frac{\partial\vec{A}^*}{\partial t})\,dS\,dt \tag{4}$$

When varied with respect to $\vec{A}$ and ϕ, respectively, the full Lagrangian then gives Eq. (5) and Eq. (6).

$$\epsilon c^2\hat{n}\times(\nabla\times\vec{A}) = (\nabla\phi + \frac{\partial\vec{A}}{\partial t})\cdot Y \tag{5}$$

$$\epsilon(\nabla\phi + \frac{\partial\vec{A}}{\partial t})\cdot\hat{n} + \nabla\cdot(\frac{\nabla\phi\cdot Y}{i\omega} + \vec{A}\cdot Y) = 0 \tag{6}$$

Note the boundary conditions are imposed on the fields, not the potentials. This is clearer when writing Eq. (5) in terms of the fields, as in Eq. (7). From this we see that Y is a dyadic representing the conductance on the boundary. It cannot have any component normal to the boundary surface. As $Y \to \infty$, a perfect electric wall is enforced, while for $Y = 0$, we are back at the magnetic wall boundary condition.

$$\hat{n}\times\vec{B}_t = -\vec{E}_t\cdot Y \tag{7}$$

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STEADY STATE, SOURCE FREE EIGENMODE SOLVER

We consider first the simple case of an eigenmode solver to solve for the frequency and field distribution of modes in a source free problem. In this case, the Lagrangian reduces to Eq. (8), where we have eliminated the integral over time by taking the Fourier transform and are now working in the frequency domain.

$$\mathcal{L}_{\mathrm{w}} = \frac{\epsilon}{2}\int |\nabla\phi_w + i\omega\vec{A_w}|^2 - c^2|\nabla\times\vec{A_w}|^2\, dv + \frac{1}{i\omega}\int (-\nabla\phi_w - i\omega\vec{A_w})\cdot Y(-\nabla\phi_w^* + i\omega\vec{A_w}^*)\, dS \quad (8)$$

In the interest of brevity, we will drop the subscript with the assumption that we are working in the frequency domain for the rest of this section. Discretizing the solution space, we can write ϕ and $\vec{A}$ in terms of a linear combination of basis functions which span the solution space:

$$\phi(\vec{x}) = \sum_i \phi_i \xi_i(\vec{x}) \quad (9)$$

$$\vec{A}(\vec{x}) = \sum_i \vec{A}_i \xi_i(\vec{x}) \quad (10)$$

A typical set of basis functions are the nodal basis functions: $\xi_i(\vec{x}_j) = \delta_{ij}$ where $\vec{x}_j$ is the coordinates of a node on the element. The basis functions are known a-priori so when the discretized solutions are substituted into the Lagrangian, we obtain the matrix equation in Eq. (11). Here $\underline{u}$ is the approximate solution, $\underline{u} = [\phi_1\phi_2, ...\vec{A}_1, \vec{A}_2, ...]$.

$$\mathcal{L}_{\mathrm{discrete}} = \underline{u}\mathbf{L}\underline{u}^{\mathrm{T}} \quad (11)$$

L can be analytically or numerically calculated according to the element geometry and basis functions selected. Varying this lagrangian amounts to independently taking the derivative of Eq. (11) with respect to all coefficients $\partial\underline{u} = (\partial u_1, \partial u_2, ...)$, resulting in the system of equations:

$$\mathbf{L}\underline{u}^{\mathrm{T}} = 0 \quad (12)$$

A Quadratic Eigenvalue Problem

Looking closer at $\mathcal{L}_{\mathrm{w}}$, we note an interesting issue that arises when solving for the potentials instead of the fields. As mentioned previously, the Helmholtz wave equation approach has $\vec{E}$ and $\vec{B}$ decoupled from each other and each can be solved independently. In this case, the system of equations can be written as a generalized eigenvalue problem where the eigenvalue $\lambda = \omega^2$ and the eigenvector, $\underline{u}$, corresponds to the approximate $\vec{E}$ or $\vec{B}$ field: $(\mathbf{M}\lambda + \mathbf{K})\underline{u} = 0$. These problems are ubiquitous and there exist many highly optimized linear algebra libraries capable of solving them numerically, for both dense and sparse matrices.

If the Coulomb or Lorentz Gauge are not explicitly selected prior to taking the variation of $\mathcal{L}$, ϕ and $\vec{A}$ remain coupled, introducing a new matrix term to the system of equations: $(\mathbf{M}\omega^2 + \mathbf{C}\omega + \mathbf{K})\underline{u} = 0$. **C** consists of the terms arising from $\nabla\phi\cdot i\omega\vec{A}^* + c.c$ and the boundary surface integral in Eq. (8). This is now a quadratic eigenvalue problem and while algorithms exist for efficient numerical solution, these types of problems end up taking twice as much memory and/or time as their linear counterparts. The issue of the quadratic eigenvalue problem can be circumvented, however, as will be discussed in the next section.

SPURIOUS MODES AND GAUGE FIXING

The question of gauge fixing in the context of the finite element method leads to some interesting discussion. The Lagrangian given by Eq. (8) is invariant the gauge transformations, $\vec{A}\rightarrow\vec{A}+\nabla\psi$, $\phi\rightarrow\phi-\frac{\partial\psi}{\partial t}$, for some function ψ. This extra degree of freedom results in an infinite number of valid solutions and Eq.(12) becomes an ill defined system. In practice, this manifests itself as singular matrices in the finite element analysis.

We were thus finding experimentally that a multitude of spurious modes were appearing. These modes appear to be unrelated to the spurious modes typically associated with numerical solutions to the Helmholtz equation. Such modes have nonzero divergence and are due to mathematical properties of the Helmholtz operator [1, 2]. The spurious modes resulting from the operator **L** did not exhibit the characteristics of conventional spurious modes such as large divergence or small curl. Likely, these spurious modes were a result of the badly conditioned problem.

Therefore a gauge must be selected or enforced at some point before solving for $\underline{u}$ but the question of when to do so is intricate. If we were to choose the Lorenz gauge, $\nabla\cdot\vec{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}=0$, before taking the variation of $\mathcal{L}$ the resulting operator reduces to the same as the Helmholtz operator with its well known issue of spurious modes (discussed above). The best known solution to avoid these spurious modes is to use the Nedelec vector basis functions which are divergence free. However, as compared to using nodal basis functions, vector basis functions increase the size of the problem by n for an n dimensional problem and will complicate the particle tracking which is being implemented in conjunction. This option was thus of little interest to us.

In quantum field theory, where the Lagrangian must also be discretized (though not within a volume but over all space), one solution is to add a gauge fixing term to the Lagrangian [3]. The gauge fixing term used is of the form:

$$\mathcal{L}_{\mathrm{GF}} = -\frac{1}{2\alpha}\int |\nabla\cdot\vec{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}|^2\, dv \quad (13)$$

This constrains the allowable gauge transformations, ψ, to those where ψ satisfies the equation $\nabla^2\psi=\frac{\partial^2\psi}{c^2\partial t^2}$. This is only a partial gauge fixing, however when combined with appropriate boundary conditions on the fields (they should approach zero at infinity), the gauge becomes fully fixed.

Taking the variation of $\mathcal{L}$ with this gauge fixing term added and applying integration by parts and vector calculus,

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we obtain Eq.(14) and (15).

$$\delta_\phi \frac{\mathcal{L}}{\epsilon} = \int\int \Big((\frac{\mu}{\alpha} - 1)\nabla \cdot \frac{\partial \vec{A}}{\partial t} + \frac{\mu}{c^2 \alpha} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi - \frac{\rho}{\epsilon} \Big) \delta\phi \, dv \, dt + \int \oint (\frac{\partial \vec{A}}{\partial t} + \nabla\phi) \cdot \hat{n} \delta\phi \, ds \, dt - \frac{\mu}{\alpha} \int (\nabla \cdot \vec{A} + \frac{1}{c^2} \frac{\partial \phi}{\partial t}) \delta\phi \, dv \Big|_{t_i}^{t_f} \quad (14)$$

$$\delta_A \frac{\mathcal{L}}{\epsilon} = \int\int \Big((\frac{1}{\epsilon\alpha} - c^2) \nabla \times \nabla \times \vec{A} \delta\vec{A} + \frac{1}{\epsilon\alpha} \nabla^2 \vec{A} - \frac{\partial^2 \vec{A}}{\partial t^2} + (\frac{1}{c^2 \epsilon \alpha} - 1) \nabla \frac{\partial \phi}{\partial t} \Big) \delta\vec{A} \, dv \, dt + c^2 \int \oint \nabla \times \vec{A} \times \delta\vec{A} \cdot \hat{n} \, ds \, dt - \frac{1}{\epsilon\alpha} \int\int (\nabla \cdot \vec{A} + \frac{1}{c^2} \frac{\partial \phi}{\partial t}) \delta\vec{A} \cdot \hat{n} ds dt + \int (\frac{\partial \vec{A}}{\partial t} + \nabla\phi) \cdot \delta\vec{A} dv \Big|_{t_i}^{t_f} \quad (15)$$

A clear choice for the parameter α is thus μ, from which it can be seen that the Lorenz gauge is enforced. Experimentally, we find that all the spurious modes which appear when the gauge fixing term is not present, attributed to the ill defined system, disappear. Additionally, the generalized quadratic eigenvalue problem reduces to a linear one as the coupling terms vanish with the appropriate basis functions, improving performance and speed of solution. A comparison of the spurious modes before adding the gauge fixing term and after is shown in Fig. 1.

IMPLEMENTATION OVERVIEW

We have begun implementing this formulation in a 2D FEM solver for azimuthally symmetric problems of degree m [4]. The solver is written in C / C++ but interfaces through Mathematica. It meshes the region defined by user, applies the boundary conditions, calculates the local triangle matrices and assembles the global matrix.

At present, we have focused on the source free case for $m = 0$, for the sake of resolving the issues of gauge fixing and spurious modes. The matrices associated with $\mathcal{L}_{\text{discrete}}$ are calculated analytically for an arbitrary triangular element. The form of the resulting analytical expressions are optimized to reduce the number of operations and ported to C code for integration in the FEM solver.

CONCLUSION

We have developed a new finite element formulation for the solution of electromagnetic problems based on the Lagrangian for the electromagnetic potentials. Some of the challenges inherent in solving for the potentials instead of the fields have been discussed, including the possibility of a quadratic eigenvalue problem due to the coupling of $\vec{A}$ and ϕ and the issue of gauge invariance. A solution to both of these problems was found in the addition of a gauge fixing term to the Lagrangian, similar to that used in quantum field theory.

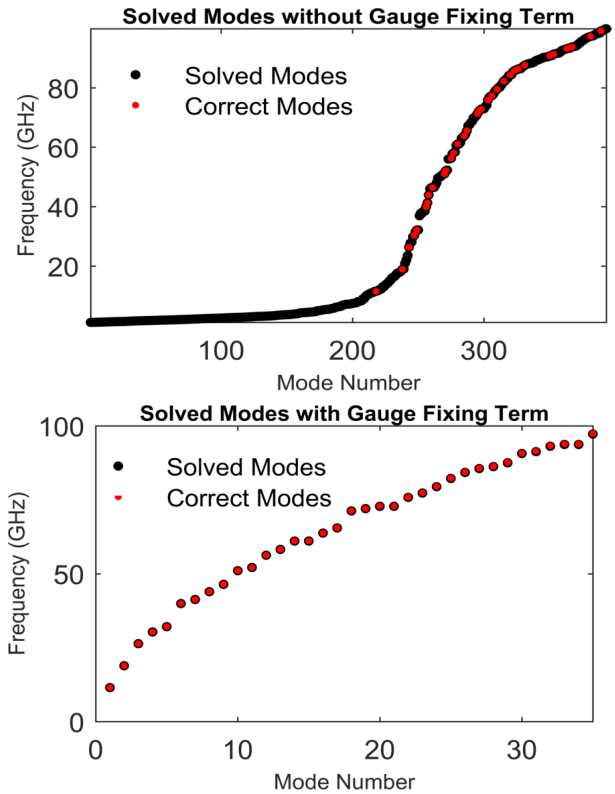

Figure 1: Frequency of the solved TM modes for a 10 mm x 10 mm pillbox cavity. Note the spurious modes when the gauge fixing term is not included compared to the bottom figure when the term is added ($\alpha = \mu_0$) and the solved modes correspond to physical modes in all cases

This formulation is particularly beneficial in that the final result has none of the spurious modes inherent to numerical solutions of the Helmholtz equation while still allowing us to work with nodal basis functions instead of the more computationally costly vector element basis functions.

Additionally, the formulation lays the groundwork for future work on simulating the beam-wave interaction through the natural accounting of the beam-wave interaction. In conjunction to implementing this beam-wave interaction, we are now working on the general case for m.

REFERENCES

[1] S. Caorsi *et al.*, "On the Convergence of Galerkin Finite Element Approximations of Electromagnetic Eigenproblems," *Siam. J. Numer. Anal.*, vol. 38, no. 2 p. 580, 2000.

[2] I. Tsukerman, "Spurious Numerical Solutions in Electromagnetic Resonance Problems," *IEEE. Trans. Magn.*, vol. 39, no. 3 p. 1405, May, 2003.

[3] C. Guigg, "Strong Interactions Among Quarks," in *Gauge Theories of the Strong, Weak, and Electromagnetic Interactions*, Princeton, USA: Princeton University Press, 2013, pp. 295.

[4] A. Vrielink, M. Nasr and S. Tantawi, "A 2D finite element solver for electromagnetic fields with m-fold azimuthal symmetry," presented at the 8th Int. Particle Accelerator Conf. (IPAC'17), Copenhagen, Denmark, May 2017, paper WEPIK112, this conference.