A Classical Field Theory Formulation for the Numerical Solution of Time Harmonic Electromagnetic Fields

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Abstract—Finite element representations of Maxwell's equations pose unusual challenges inherent to the variational representation of the “curl-curl” equation for the fields. We present a variational formulation which solves for the four-potential instead, based on classical field theory. Borrowing from quantum electrodynamics, we modify the Lagrangian by adding an implicit gauge-fixing term. This reformulation explicitly accounts for Gauss’ law through the coupling between \( \phi \) and \( \rho \), and enables the use of nodal basis functions instead of edge elements for time-harmonic problems. We demonstrate how this formulation, adhering to the deeper underlying symmetries of the four-dimensional covariant field description, provides a highly general, robust numerical framework.

Index Terms—Electromagnetic (EM) fields, finite element (FE) method, Lagrangian mechanics.

I. INTRODUCTION

As engineers and physicists seek to model increasingly complex electromagnetic systems, from radio-frequency power sources to integrated photonics, the need for efficient and robust full-wave, first-principles numerical field solvers is growing. Finite element (FE) methods are a natural solution enjoying widespread use.

In electromagnetic (EM) problems, the variational formulation driving the FE method presents unique challenges which impede the computational efficiency and accuracy of existing solvers. For time harmonic problems where the fields oscillate at angular frequency \( \omega \), \( \tilde{E}(\vec{r}, t) = \Re [\tilde{E}(\vec{r}) e^{i \omega t}] \), this variational expression is given by (1). Here, \( \mu_\perp \) and \( \epsilon_r \) are the relative permeability and permitivity, \( k_0 \) is the wave number in free space, \( Z_0 \) is the intrinsic impedance of free space, and \( \vec{J} \) is the current density [1]

\[
F = \int_{\Omega} \left( \frac{1}{\mu_\perp} |\nabla \times \vec{E}|^2 - k_0^2 \epsilon_r |\vec{E}|^2 \right. \\
\left. + i k_0 Z_0 (\vec{E}^* \cdot \vec{J} - \vec{E} \cdot \vec{J}^*) \right) \, dV. 
\]

The primary challenge consists in enforcing the divergence constraint associated with Gauss’s law, \( \nabla \cdot \vec{E} = -\frac{\rho}{\epsilon_0} \), while ensuring adequate freedom in the basis functions to model discontinuities in the fields [2], [3]. These two requirements conflict in standard nodal element finite-element method (FEM), employed successfully in fields from fluid mechanics to structural mechanics.

Significant research over the past several decades has focused on resolving these issues through modifications to (1) or the FE framework. We present here a fundamentally different approach which bypasses the issue entirely. The classical field theory Lagrangian is applied to solve for the four-dimensional (4-D) covariant four-potential \( A^\mu \). This is given in the framework of differential geometry by (2). The first two terms constitute the classical Lagrangian and the final term, multiplied by the scalar \( \frac{1}{2\mu_\perp} \), is a gauge-fixing term adapted from quantum electrodynamics

\[
\mathcal{L} = -\frac{1}{2\mu_\perp} dA \wedge *dA + A \wedge J - \frac{1}{2\mu_\perp} d* A \wedge *d A. 
\]

Here, \( \mu \) is the magnetic permeability, \( A = A_\| dx^\nu \) is the 4-D differential 1-form, \( A^\nu = (\frac{\partial}{\partial x}, \vec{A}) \) is the four-potential consisting of the electrostatic potential \( \phi \) and magnetic vector potential \( \vec{A} \), and \( J \) is the electric current 3-form. In this article, we use the metric signature (+ − − −).

As both \( \rho \) and \( \vec{J} \) are captured in the interaction term \( A \wedge J \), (2) explicitly accounts for both Ampere’s law and Gauss’ law, unlike (1). This provides a unified formulation applicable from dc to high frequency, alleviating the need for the mixed FE schemes used in conventional EM-FEM at dc and low frequency. This also renders the formulation insusceptible to the well known issue of spurious nonsolenoidal solutions resulting from the failure of (1) to enforce Gauss’ law. The best existing solution, tree-cotree gauging, is robust but computationally costly as a spanning tree must be computed for a given mesh and set of boundary conditions. Additionally, the resulting linear system tends to be ill conditioned with condition number depending strongly on the tree selected.

The second remarkable feature of this formulation is that it can be used in conjunction with standard nodal FEM instead of requiring edge elements, presenting significant benefits for multiscale and multiphysics simulations. The same framework, including preprocessing and postprocessing, can be applied to all physical quantities solved for, and interpolation error is avoided by solving for all quantities at the same location. Methods developed in mature fields (structural mechanics, computational...
fluid dynamics) to accelerate the solver and improve accuracy are directly applicable.

We begin in Section II with the background and motivation for this work before presenting the classical field theory Lagrangian in Section III. We demonstrate how this formulation is related to existing $\vec{A} - \phi$ approaches obtained by substituting the potentials into (1), yet differs in a few critical points which ensures a fully 4-D formulation and enables the use of nodal elements. Finally, Sections IV and V introduces a proof of concept implementation and demonstrates the validity of the formulation with benchmarking results compared to a state-of-the-art edge element field solver.

II. BACKGROUND

We motivate this idea by considering how the challenges inherent to (1) are currently resolved. Enforcing the divergence constraint was initially addressed by adding a regularization term of the form $s(\nabla \cdot \vec{E})^2$ to (1), with limited success [4]–[7]. While the regularization term eliminates spurious nonsolenoidal modes in the solution spectrum, the regularized formulation fails to converge to the correct solution for problem geometries with sharp or re-entrant corners. The explanation for this failing was only recently understood—when nodal basis functions are used in conjunction with the regularization term, the approximate solution space spanned is overly restrictive on nonconvex domains [8]. When singularities in the field exist, such as at sharp corners, it can be shown that the missing subspace consists of the gradients of solutions to Laplace’s equation on the same domain [9], [10]. Instead of converging to the correct solution with field singularities, the solution obtained will be the projection of the correct fields on the smooth approximate solution space.

Two approaches exist to resolve this issue. One can either supplement the nodal basis functions with additional singular or nonconforming functions [11]–[13], or relax the regularization term near the singularity [14]–[16]. The former requires computing the coupling between the nodal basis and the additional singular functions and is challenging to extend to three dimensions while the latter is a compromise between enforcing the divergence constraint over the problem domain and not completely restricting the subspace spanned by gradients.

A more robust solution arises by formulating electromagnetism in the language of differential geometry. In 3-D Euclidean space, $\vec{E}$ (and $\vec{A}$ in the Coulomb gauge) are both differential 1-forms which should be expanded not on nodes but on edges. This led to the development and widespread adoption of the “edge elements” for EM problems, as developed separately by Whitney [17] and Nédélec [18]. By their construction, only tangential continuity is imposed at the faces between elements, resolving the issue of modeling field discontinuities at interfaces and boundaries. However, while the edge elements are divergence-free locally, the discontinuity in the normal field at element interfaces allows for solutions that are not divergence-free globally. The space spanned by edge elements divides into the desired space of weakly divergence-free fields and its codomain, the kernel of the curl operator (purely gradient functions in topologically trivial domains) [19], [20]. There are methods to extract the gradient field so as to span only the divergence-free fields, such as the tree-cotree method [21]–[24]. However, choosing an optimal tree is challenging and poor conditioning of the resulting linear system is a common issue [25]–[28].

III. COVARIANT 4-D FIELD THEORY FORMULATION

A. Insight From Differential Geometry

Compared to the 3-D formulation, EM theory is encoded much more succinctly by differential geometry in 4-D Minkowski space, where deeper underlying structure is made explicit, such as gauge and Lorenz invariance. For Lorenzian manifolds, the equations for the EM field tensor, $\mathbf{F} = d\mathbf{A}$, are given by (3) and (4). As defined in Section I, $\mathbf{A} = A_\nu dx^\nu$ is the 4-D differential 1-form, $A^\nu = (\frac{x^\nu}{c}, \mathbf{A})$ is the four-potential, and $\mathbf{J} = -\rho dx \wedge dy \wedge dz + j_x dt \wedge dy \wedge dz + j_y dt \wedge dx \wedge dz + j_z dt \wedge dx \wedge dy$ is the current 3-form.

$$d\mathbf{F} = 0 \quad (3)$$
$$d * \mathbf{F} = \mathbf{J} \quad (4)$$

The classical field theory Lagrangian which encodes these equations, written in terms of $\mathbf{A}$, is given as

$$\mathcal{L} = \frac{1}{2\mu} d\mathbf{A} \wedge *d\mathbf{A} + \mathbf{A} \wedge \mathbf{J}. \quad (5)$$

In the covariant treatment, it is natural to work with $\mathbf{A}$ as opposed to $\mathbf{E}$ and $\mathbf{B}$, the 3-D components of the two-form $\mathbf{F}$. In this case, (3) is automatically satisfied as $d^2 = 0$. Additionally, the charge density $\rho$, which does not enter into the conventional variational expression for the fields given by (1), is accounted for in (5) through $\mathbf{J}$.

Applying the variational formulation given by the action of (5) in the FE method, we first consider the appropriate elements over which to expand the solution $\mathbf{A}$. As in 3-D Euclidean space, where there is a duality between 1-forms and edges, in a 4-D mesh, the 1-form $\mathbf{A}$ should be expanded using edge elements. This is an intriguing idea to pursue for transient numerical analysis, where one could envision using this formulation on a 4-D mesh. In the case of time harmonic problems—the focus of this work—the 4-D solution is projected onto a 3-D mesh and we find that the nodal elements provide a suitable basis.

A robust analysis of the consequences of this requires the derivation of 4-D Whitney elements and will be pursued in future work. Regardless, there are two explanations which we propose at present. First, it is clear that $\nabla \phi$ provides the missing subspace in nonconvex domains required to model the $\vec{E}$ field—the gradients of solutions to Laplace’s equation on the singular domain. Second, referring to the full derivation of the Lagrangian FE formulation and its corresponding strong form given in the appendix, within the volume it is possible to decouple the components of the four-potential. The result is a set of four Laplacian partial differential equations (PDEs) to be solved, each inherently scalar in nature and suited to expansion using nodal elements. We find, however, that even when the four-potential is not decoupled in the volume, the nodal elements work well, suggesting a more general explanation exists.
GOLD AND TANTAWI: CLASSICAL FIELD THEORY FORMULATION FOR THE NUMERICAL SOLUTION OF TIME HARMONIC EM FIELDS 247

B. Gauge Invariance and Ill-Conditioned Systems

The linear systems resulting from employing (5) in the FE method are, unfortunately, highly ill-conditioned. This should come as no surprise when considering that unlike the fields, the four potential is not uniquely defined. The Lagrangian is invariant to gauge transformations of the form $A \rightarrow A + d\phi$ where $\psi$ is a scalar 0-form. To resolve this issue, we apply a solution used to address a similar challenge in QED. In the field discretization in QED, the resulting symbolic matrices are singular due to gauge invariance. One approach to overcome this issue is through the addition of a gauge fixing term to the Lagrangian [29]

$$\mathcal{L}_{GF} = -\frac{1}{2\mu}\mathbf{d} \star \mathbf{A} \wedge \star \mathbf{d} \star \mathbf{A}. \quad (6)$$

The resulting action integral for time harmonic problems, integrated over the time dimension already, is given by (7). Here, we have expanded $\mathbf{A}$ into the conventional three-plus-one notation $(\tilde{A} + \phi)$ for ease of comparison to existing formulations and to expose some implementation challenges, which will be discussed in Section IV. As we are now working in the frequency domain, $\phi$ and $\tilde{A}$ as given as follows are complex quantities. The strong problem corresponding to (7), obtained by taking the variation of this action integral, is derived in the appendix.

$$S(\phi, \tilde{A}) = \frac{1}{2} \int \epsilon |\nabla \phi + i\omega \tilde{A}|^2 - \frac{1}{\mu} |\nabla \times \tilde{A}|^2 - \frac{1}{\mu\epsilon} |\nabla \cdot \tilde{A} - \frac{i\omega}{c^2}\phi|^2 - \rho \phi^* - \rho^* \phi + \tilde{A} \cdot \tilde{J} + \tilde{A}^* \cdot \tilde{J} \, dV \quad (7)$$

In QED, the gauge-fixing term imposes different gauges depending on the value of $\xi$. In our classical context, any $\xi \neq 0$ imposes the Lorenz gauge with residual gauge freedom $\mathbf{A} \rightarrow \mathbf{A} + d\psi$ for $\psi$ satisfying the wave equation $\nabla^2 \psi + k_0^2 \psi = 0$. By setting the components of $\mathbf{A}$ or their derivatives explicitly on the boundary, $\psi$ is forced to zero on the boundary, and hence everywhere, and $\mathbf{A}$ will be unique.

Tempting as this may be, doing so in the most straight-forward way (setting $\tilde{A}_n = 0$ and $\phi = 0$ on the boundary for a perfect electric conductor, or $\tilde{A}_n = 0$ and $\nabla \cdot \phi = 0$ for a perfect magnetic conductor) in fact decouples $\phi$ from $\tilde{A}$. This reduces the problem to two separate wave equations: (8), which is amenable to nodal elements, and (9), which reduces to the curl-curl equation for $\tilde{A}$ and must be solved via edge elements.

$$\nabla^2 \phi + k_0^2 \phi = -\frac{\rho}{\epsilon} \quad (8)$$

$$\nabla^2 \tilde{A} + k_0^2 \tilde{A} = -\mu j \quad (9)$$

On this note, we have since discovered the work of Boyse and Paulsen, who had started to develop a nodal-element-based formulation by substituting the potentials into Maxwell’s equations and applying the Lorenz gauge [30], [31]. Their weak formulation is missing some of the coupling terms that appear in the Lagrangian formulation with gauge fixing and the resulting strong form of the problem has no direct coupling between $\tilde{A}$ and $\phi$ in the volume. However, the main issue in their original formulation is precisely the application of the boundary condition scheme suggested above, decoupling $\tilde{A}$ and $\phi$. While not mentioned in the original works, a nodal implementation of the formulation will fail on nonconvex domains, as noted in [32]. Nonetheless, it is perfectly acceptable to adopt such an approach, as long as a mixed formulation is employed, with $\tilde{A}$ expanded by the edge elements.

This decoupled, mixed formulation approach has been adopted by some low-frequency solvers. In these implementations the Lorenz gauge simplifies to the usual divergence-free condition on $\tilde{A}$ and the two components are coupled only in the sense that their excitations are related through the charge continuity equation $\nabla \cdot \tilde{J} = i\omega \rho$ [33]. In this sense, it is not a fully 4-D solution.

Instead, we allow the residual gauge freedom to persist by imposing boundary conditions solely through surface integrals instead of explicit Dirichlet boundary conditions. This is not a significant drawback, as surface integrals are commonly used to implement impedance or absorbing boundary conditions in any case. The natural boundary condition in our formulation corresponds to a perfect magnetic boundary. An impedance boundary condition can be imposed through the additional surface integral given by (10). A perfect electric boundary is imposed in the limit where the conductance, directly proportional to $\gamma$ is large. For further discussion of the boundary condition imposed by (10) and for a definition of $\gamma$ in the context of our implementation, please see the appendix.

$$S_Z = \gamma \int_{\partial \Omega} |\hat{n} \times (-\nabla \phi - i\omega \tilde{A})|^2 \, dS \quad (10)$$

In contrast to the mixed formulations, the resulting solution is not a simple superposition of independent solutions for $\tilde{A}$ and $\phi$, but a self-consistent solution for $\mathbf{A}$ in its entirety, as is demonstrated in Section V. This, in conjunction with the gauge-fixing term which regularizes the problem, is what enables the use of nodal elements in the four-potential formulation compared to existing $\tilde{A} - \phi$ formulations [23], [33]–[36]. Boyse and Paulsen arrived at a similar conclusion with their Maxwell-based $\tilde{A} + \phi$ formulation, implementing an impedance boundary condition in a later paper which they then demonstrated working on a 2-D wedge geometry [37].

Finally, we conclude this section by introducing a new coefficient for the gauge-fixing term

$$\alpha = \frac{1}{\xi}. \quad (11)$$

This is both for the sake of brevity, as the coefficient of the gauge-fixing terms is referred to often in the implementation and results section, and also as we are interested in plotting solution properties as a function of $\alpha$ near zero.

C. Gauss’ Law

While the ability to use nodal elements is a nice benefit, the primary motivation for our adoption of the Lagrangian formulation is the fully general treatment of the source terms provided.
When source distributions are driving the fields, such as in particle-in-cell codes used in plasma and accelerator physics, correction schemes must be applied to either the field calculation or the source distribution to bound the error in $\nabla \cdot \tilde{E}$ and avoid numerical instabilities [38]–[42]. For stationary and low-frequency or broadband problems, such as in electro-quasistatics and integrated circuit design, mixed FE solutions combined with tree-cotree splitting of the mesh and/or Lagrange multipliers are commonly applied to account for the contributions of $\rho$ and $\tilde{J}$ in the static limit separately [33], [41], [43]. In contrast, the four-potential formulation provides a unified framework to capture the contribution of $\rho$ at dc and high frequency, even when charge conservation is not discretely satisfied, resolving both issues.

In the appendix, we provide the full derivation of the strong form corresponding to (7) or, in the language of variational calculus, the Euler–Lagrange equations resulting from the variation of the Lagrangian. The following give the resulting equations imposed in the volume (there are also surface terms which are provided in the appendix):

$$\alpha n^2 k_0^2 \phi + \nabla^2 \phi - ik_0(\alpha - 1)\nabla \cdot \tilde{A} = -\frac{\rho}{\epsilon}$$  \hspace{1cm} (12)

$$n^2 k_0^2 \tilde{A} + \nabla^2 \tilde{A} + (\alpha - 1)\nabla(\nabla \cdot \tilde{A} + i\frac{\omega}{c^2} \phi) = -\mu \tilde{J}.$$  \hspace{1cm} (13)

Equation (12) is the result of the variation with respect to $\phi$ while (13) arises through the variation with respect to $\tilde{A}$. With the Lorentz gauge implicitly imposed through the gauge-fixing term, regardless of the residual gauge, these equations reduce to Gauss’ law and Ampere’s law in this gauge. Thus, unlike in (1), both equations are independently satisfied by the solution which minimizes (7), even in the case where discrete charge conservation is not guaranteed.

Not only does the solution explicitly satisfy Gauss’ law, but the use of the nodal elements means it can do so elementwise as well as globally. This is in contrast to the lowest order edge elements, which are divergence-free within each element—any nonzero divergence in the fields arises only through discontinuities in the normal component of the field between elements of the mesh. Furthermore, there is significant flexibility offered by the fact that both $\rho$ and $\tilde{J}$ can be used to drive the fields.

Both of these features are beneficial in modeling problems with significant space charge, whether for low-frequency applications where $\rho$ becomes important in the static limit or, as in our motivation for pursuing this approach, in the modeling of high-frequency power sources where time harmonic components of the space charge contribute strongly to the fields even at high frequencies.

IV. COMPUTATIONAL IMPLEMENTATION

As a proof of concept, we have implemented this formulation for 2.5-D azimuthally symmetric fields, solving on a 2-D mesh and accounting for the azimuthal dependance of the fields, of the form $e^{im\theta}$, a priori. A few unique challenges arise in the implementation of the Lagrangian FE formulation. The issue of enforcing boundary conditions through surface integrals instead of having the option of explicitly setting Dirichlet boundary conditions was discussed in Section III-B. The other significant difference relative to the curl-curl formulation is the presence of terms linear in $k_0$.

In FE EM analysis, there are two types of problems which are of interest—eigenmode analysis and driven problems. In driven problems, the driving frequency is known so that only the fields need to be computed. In the eigenmode analysis, the resonant frequencies (eigenvalues) and corresponding eigenvectors are calculated. The discretized Lagrangian is composed of three FE matrices $M, C, K$, and the resulting matrix equation is a generalized quadratic eigenvalue problem (QEP) where we solve for $\tilde{k}_0$, the approximate resonant frequency, and $a$, the coefficients of the approximate solution over the discretized space

$$\left(M\tilde{k}_0^2 + C\tilde{k}_0 + K\right)a = 0.$$  \hspace{1cm} (14)

It is the coupling between $\tilde{A}$ and $\phi$, appearing in the matrix $C$, that results in a QEP instead of the regular generalized eigenvalue problem of the curl-curl equation. QEPs are common in FE problems, for example, in modeling damped structural resonances and a significant body of work exists on the topic, including a comprehensive review paper [44].

We implemented the sparse nonlinear eigenvalue solver, NLFEAST [45], a contour-integral-based solver where we constructed the kernel specifically for our QEP. Our implementation has proven robust, agreeing with the direct solver for small problem sizes where a comparison was possible, and scalable up to matrix sizes on the order of $10^6$ (we did not test beyond this as for a 2-D mesh, this is a very dense mesh). The condition number of the eigenvalues, as defined in [44], are reasonable and uncorrelated to problem size. The conditioning does depend weakly on the gauge-fixing term and the need for the gauge-fixing term becomes immediately clear from the singularity in the condition number when it is not included, as will be shown in Section V.

The driven problem employs the same $M, C$, and $K$ matrices, but $\tilde{k}_0$ is set by the frequency of the driving source terms and $a$ is determined by solving the resulting linear system

$$\left(M\tilde{k}_0^2 + C\tilde{k}_0 + K\right)a = \tilde{J}.$$  \hspace{1cm} (15)

For this, we use the Intel Math Kernel Libraries, and in particular, the PARDISO solver. We have tried direct and iterative solvers and found both to be equally effective for the moderate problem sizes we have been working with so far.

Future work will look to scale the implementation to 3-D meshes and thus, much larger matrices. Here, a more advanced solver and the employment of a preconditioner will likely be beneficial. We expect NLFEAST or a similar contour integral solver will still be the optimal choice for the eigenmode analysis.

V. NUMERICAL RESULTS AND BENCHMARKING

We have benchmarked the Lagrangian formulation with respect to the edge element curl-curl formulation over several 2.5-D and 3-D examples. The results demonstrate that our proposed approach is not susceptible to spurious modes and
provides the correct solutions over a range of convex and non-convex geometries using the nodal elements. Furthermore, the accuracy of these results is comparable to that obtained using a state-of-the-art edge element solver. This section thus demonstrates that the Lagrangian approach is a suitable alternative to conventional edge element solvers, with the advantages of being directly applicable in a standard nodal FEM solver and not needing tree-cotree gauging. For comparison, we use ANSYS HFSS [46] and COMSOL [47], commercially available edge-element EM-FEM solvers widely adopted within the industry and academia. However, ANSYS HFSS is a purely 3-D solver, so only COMSOL is used in benchmarking the 2.5-D problems on a 2-D mesh. While our implementation uses nodal Lagrange elements and HFSS and COMSOL are using edge elements, in all cases, quadratic elements were employed.

In the convergence plots and tables in this section, we define the error as follows. For the frequency and wavenumber, the error is computed as \( \Delta f = \frac{f_{\text{ theor}} - f_{\text{choice}}}{f_{\text{choice}}} \) and \( \Delta k_0 = \frac{k_0 - k_{0, \text{ theor}}}{k_{0, \text{ theor}}} \) if a theoretical solution exists. If not, we use instead the solution on a mesh that is roughly twice as fine as those plotted as the reference value. For the fields, we calculate the L2 norm of the field error over the problem domain for each field component, then take the average over all six field components. Sections V-A and V-B provide the benchmarking results compared with existing approaches while in Section V-C, we explore numerical conditioning and robustness through further experimental results. Finally, in Section V-D we demonstrate the flexibility offered by the Lagrangian formulation in accounting for charge and current density.

A. 2.5-D Examples

The examples shown in the following are azimuthally symmetric, solved in a cylindrical coordinate system \((r, \theta, z)\) with an azimuthal dependence of the form \(e^{im\theta}\), as given by (16). As this dependence is known \textit{a priori}, these modes can be solved on a 2-D mesh with \(\theta\) out of plane. In the following, all figures of mode profiles are thus cross-sectional views of the full structure in the \((z, r)\) plane.

\[
\tilde{E}(\vec{r}, t) = \text{Re}[\tilde{E}(\vec{r})e^{i\omega t + im\theta}]
\]  

(16)

For monopole modes \((m = 0)\), the fields split into modes which can be represented by \(A_0\) alone (transverse electric or TE), or as a combination of \(A_z, A_r\), and \(\phi\) (transverse magnetic or TM). The TE modes are not susceptible to the challenges discussed previously and are already often solved using nodal basis functions, so we focus only on TM modes for \(m = 0\). We also demonstrate examples of dipole \((m = 1)\) and quadrupole modes \((m = 2)\). In this case, the problem is 4-D—all components of the four-potential couple to each other and are solved for.

We begin with a cylindrical cavity, the results of which can be compared to an analytical solution. Fig. 1 shows the cross-sectional problem geometry and the mode profiles for the TM_{011} mode with a perfect magnetic boundary condition. Only the components of \(E_r\) and the full vector field plot are shown for the sake of brevity. Two distinct solutions for the four-potential are shown, corresponding to different values of the gauge-fixing coefficient \(\alpha\) defined in (11). Changing \(\alpha\) numerically perturbs the system, producing a solution with a different residual gauge \(\psi\). Nonetheless, the resonant frequencies and fields calculated from the different solutions for the four-potential correspond to the same mode.

An interesting consequence of calculating different \(A\) for the same mode is that the numerical error is different in each case, as demonstrated by Fig. 2. As the mesh is refined, all solutions converge to the same frequency and fields. Plotting this convergence, now for only a few values of \(\alpha\), Fig. 3 demonstrates similar convergence characteristics for both the nodal and edge elements. The slopes of the linear fits match those predicted from theory for second-order elements, converging as \(O(h^4)\) where \(h\) is the maximum mesh edge length. The results for the first few modes are summarized in Table I for both a coarse and fine mesh, depicted in Fig. 4.

A possible downside in solving for the four-potential is the field calculation. This requires taking derivatives of the FEM solution which do not converge at the same rate as the solution itself. This is also an issue with the curl-curl formulation, as the magnetic field must be calculated from the solution for the electric field or vice-versa. There are methods to resolve or mitigate this issue, for example, the superconvergent patch recovery technique often employed to compute stress in structural
Fig. 3. Convergence of the frequency for the mode in Fig. 1 with mesh size $h_{\text{mesh}}$. The slopes of the linear fits are 3.66 (COMSOL), 3.81 ($\alpha = 0.1$), 3.96 ($\alpha = 1$), and 3.90 ($\alpha = 10$).

Fig. 5. Convergence of the fields for the TM$_{011}$ mode with mesh size $h_{\text{mesh}}$. The slopes of the linear fits are 1.99 (COMSOL), 2.14 ($\alpha = 0.1$), 2.69 ($\alpha = 1$), and 2.43 ($\alpha = 10$).

**Table I**

| Mode | $k_0,\text{theor}$ | COMSOL | Nodal, $E$ | Nodal, $A$ |
|------|-----------------|--------|------------|-----------|
| 1    | 4.95495         | 8.45 $\cdot 10^{-4}$ | 5.52 $\cdot 10^{-4}$ | 2.42 $\cdot 10^{-3}$ |
| 2    | 7.35937         | 2.53 $\cdot 10^{-3}$ | 7.34 $\cdot 10^{-3}$ | 1.24 $\cdot 10^{-2}$ |
| 3    | 7.68688         | 5.17 $\cdot 10^{-3}$ | 2.99 $\cdot 10^{-2}$ | 8.37 $\cdot 10^{-3}$ |
| 4    | 9.41790         | 3.15 $\cdot 10^{-2}$ | 7.28 $\cdot 10^{-3}$ | 1.65 $\cdot 10^{-2}$ |
| 5    | 10.17391        | 6.67 $\cdot 10^{-3}$ | 8.88 $\cdot 10^{-3}$ | 1.73 $\cdot 10^{-2}$ |
| 6    | 10.64749        | 2.59 $\cdot 10^{-2}$ | 1.09 $\cdot 10^{-2}$ | 2.31 $\cdot 10^{-2}$ |

The meshes are shown in Fig. 4.

Fig. 4. Coarse and fine mesh used in Table I.

Fig. 6. Incorrect solution for the fundamental TM mode of an L-shaped cylindrical cavity with a nodal FE solver based on the curl-curl formulation. No singularity is evident at the re-entrant corner.

As evident in Table I, for the convex geometry of the cylindrical cavity, the nodal curl-curl field solver is capable of providing the correct solution. We consider now a nonconvex hull, that of an L-shaped cylindrical cavity. While nodal-element-based solvers using the conventional curl-curl formulation fail on this geometry, the four-potential formulation does not. This is illustrated in the field profile of the fundamental mode with a perfect electric boundary condition for the L-shaped cavity, given by Figs. 6 and 7. Nodal elements are used in both cases but whereas the conventional curl-curl nodal formulation does not resolve the singularity in the fields (see Fig. 6), the four-potential formulation is able to capture the discontinuity through the gradient of $\phi$ (see Fig. 7). Table II compares the wavenumber computed for this fundamental mode in addition to the next four modes, also demonstrating the failure of the nodal field solver.

In Fig. 9, the convergence of the frequency for the fundamental mode is plotted as a function of the number of degrees of freedom solved for. The convergence of the fields corresponding to this mode are plotted in Fig. 10. Instead of plotting as a function of mesh size, where we do not expect to obtain a theoretical rate of convergence due to the singularity in any case, we plot as a function of problem size to illustrate another perhaps counter-intuitive result. The absolute accuracy relative to problem size is comparable despite the additional degree of freedom used in the four-potential formulation. This is because edge elements comparable results with those computed by COMSOL. The convergence of the fields for the mode in Fig. 1 are given by Fig. 5.
require more degrees of freedom than nodal elements for the same convergence order [1], [49], in part due to the additional
degrees of freedom per mesh element and in part because there
are many more edges than nodes in a mesh.

In addition to field singularities due to singular boundaries
and re-entrant corners, the four-potential formulation can model
discontinuities at material interfaces. A nodal field solver is
not able to do this without special treatment to accommodate
the jump in the normal field (dual nodes on the boundary,
for example) [1]. Fig. 11 shows the field profile for a tapered
dielectric lined cavity, for example.

Finally, we end the 2.5-D examples with two more realistic
problems, starting with a spherical cavity with a complex
impedance boundary condition. As we have not yet implemented
curvilinear or isoparametric elements, the convergence rate in
this case is dominated by the extent to which the curved boundary
is approximated by a polygon. The results shown are for the
TM<sub>222</sub> mode (TM with respect to \( \rho = \sqrt{r^2 + z^2} \)). Figs. 12 and
13 plot the mode profile and resulting fields. The convergence
with mesh and problem size are shown in Fig. 14. Both are
plotted to demonstrate that while the convergence with mesh is

| Mode | COMSOL | Nodal, \( \vec{E} \) | Nodal, \( \vec{A} \) |
|------|--------|------------------|------------------|
| 1    | 2.53822| 3.83734          | 2.53537         |
| 2    | 5.14864| 5.36979          | 5.13811         |
| 3    | 5.92637| 6.12445          | 5.95903         |
| 4    | 6.84954| 7.07802          | 6.89780         |
| 5    | 8.21349| 8.32246          | 8.36786         |

The meshes are shown in Fig. 8.

Fig. 7. FE solution for the fundamental TM mode of an L-shaped cylindrical
 cavity, solving for \( \phi, A_x, \) and \( A_z \) are continuous but the singularity is
captured in the computed fields through \( \nabla \phi \).

Fig. 8. Coarse and fine mesh used in Table II.

**TABLE II**

| Mode | COMSOL | Nodal, \( \vec{E} \) | Nodal, \( \vec{A} \) |
|------|--------|------------------|------------------|
| 1    | 2.54585| 3.61850          | 2.54583         |
| 2    | 5.15080| 5.32501          | 5.15078         |
| 3    | 5.93023| 6.02633          | 5.93022         |
| 4    | 6.84907| 7.01266          | 6.84904         |
| 5    | 8.20267| 8.33694          | 8.20265         |

The slopes of the linear fits are \(-0.83\) (COMSOL), \(-0.86\) (\( \alpha = 0.1 \)),
\(-0.85\) (\( \alpha = 1 \)), and \(-0.83\) (\( \alpha = 10 \)).
Fig. 11. FE solution for the fundamental TM mode of a dielectric-lined cavity with $\epsilon_r = 1.5$ above the thick back line. The resonant frequency is $f_0 = 214.051$ MHz compared to 214.054 MHz in COMSOL.

Fig. 12. TM$_{222}$ mode of a spherical cavity with a complex impedance boundary condition—FE solution for the four-potential. The mesh used is shown as an overlay in the plot for $\phi$.

Fig. 13. Computed fields for the mode in Fig. 12.

Fig. 14. Convergence of the resonant frequency for the spherical cavity mode in Fig. 12. (a) Convergence with mesh size $h_{\text{mesh}}$. The slopes of the linear fits are 2.34 (COMSOL), 2.34 ($\alpha = 0.1$), 2.36 ($\alpha = 1$), and 2.44 ($\alpha = 10$). (b) Convergence with problem size $n_{\text{DOF}}$. The slopes of the linear fits are $-1.19$ (COMSOL), $-1.19$ ($\alpha = 0.1$), $-1.2$ ($\alpha = 1$), and $-1.25$ ($\alpha = 10$).

Fig. 15. Cut-away view of a re-entrant cavity.

essentially identical in both cases, the four-potential formulation actually results in a slightly smaller problem size.

The final 2.5-D example considered is of a re-entrant cavity, a more complex shape commonly encountered in accelerators and RF sources, shown in 3-D in Fig. 15. Fig. 16 plots the convergence of the TM$_{110}$ mode. Here, we once again find similar performance between the new four-potential formulation and the edge element solver. Due to the particular geometry and mesh layout, in this case, the edge elements required roughly 1.2 times more degrees of freedom to model the same problem.
GOLD AND TANTAWI: CLASSICAL FIELD THEORY FORMULATION FOR THE NUMERICAL SOLUTION OF TIME HARMONIC EM FIELDS

Fig. 16. Convergence of the resonant frequency for the re-entrant cavity in Fig. 15. (a) Convergence with mesh size \( h_{\text{mesh}} \). The slopes of the linear fits are 2.68 (COMSOL), 2.68 (\( \alpha = 0.1 \)), 2.68 (\( \alpha = 1 \)), and 2.68 (\( \alpha = 10 \)). (b) Convergence with problem size \( n_{\text{DOF}} \). The slopes of the linear fits are −1.51 (COMSOL), −1.52 (\( \alpha = 0.1 \)), −1.52 (\( \alpha = 1 \)), and −1.52 (\( \alpha = 10 \)).

Table III

| Mode | \( k_{0,\text{theor}} \) | COMSOL | HFSS | Nodal, A |
|------|-----------------|--------|------|---------|
| 1 (3) | 4.442288 | 1.31 \times 10^{-3} | 8.47 \times 10^{-4} | 5.45 \times 10^{-3} |
| 2 (2) | 5.44140 | 3.34 \times 10^{-3} | 1.28 \times 10^{-3} | 6.98 \times 10^{-3} |
| 3 (6) | 7.02481 | 1.52 \times 10^{-3} | 2.72 \times 10^{-3} | 2.63 \times 10^{-2} |

Table IV

Wavenumber \( k_0 \) of the First Several Modes of a Fichera Corner Problem

| Mode | Bramble et al. [51] | COMSOL | HFSS | Nodal, A |
|------|---------------------|--------|------|---------|
| 1 | 3.23432 | 3.30214 | 3.29843 | 3.39252 |
| 2 | 5.88267 | 5.88009 | 5.80777 | 5.93006 |
| 3 | 5.88371 | 5.89004 | 5.88330 | 5.95513 |
| 4 | 10.6789 | 10.62856 | 10.63372 | 10.62203 |
| 5 | 10.6832 | 10.67236 | 10.64633 | 10.75643 |
| 6 | 10.6945 | 10.77349 | 10.65130 | 10.81040 |
| 7 | 12.3953 | 12.43494 | 12.44877 | 11.81689 |
| 8 | 12.3723 | 12.48868 | 12.46236 | 12.01566 |

The meshes are shown in Fig. 17. The HFSS mesh was different, but the resolution was set to obtain approximately the same problem size.

B. Three-Dimensional Examples

For 3-D problems, we first consider a rectangular cavity. In a similar manner to the 2.5-D examples, Table III compares the results for the first several modes using edge elements, the conventional nodal element curl-curl formulation, and the proposed four-potential formulation. In 3-D, the nodal field solver (using the curl-curl formulation with penalty term) performed very poorly and is not included in the comparison.

The second problem presented is that of the Fichera corner: \([−1,1]^3 \setminus [−1,0]^3\). While no analytical solution exists for comparison, Table IV gives the computed wavenumber for the meshes shown in Fig. 18, allowing a comparison with the values obtained by existing strategies [32], [50], [51]. As with the L-shaped cylindrical cavity in Fig. 7, the conventional curl-curl nodal formulation would not produce the correct results due to the singularity at the inner corner.

Because of the highly singular nature of the problem, it is difficult to evaluate which result is more correct; we provide the results obtained by Bramble et al. for comparison [51], but these
are results for a specific mesh and element type. The agreement between COMSOL and HFSS is not surprising given they use the same edge elements, such that the resulting linear system should be essentially identical. Relatively good agreement between the four approaches is nonetheless obtained in the case of the fine mesh (as compared with, for example [32]).

C. Robustness

There are two particular aspects to robustness that we consider here—numerical conditioning and the question of spurious modes. A rigorous theoretical analysis is beyond the scope of this article but we have investigated these issues experimentally. For the eigenmode analysis, we use the definition of condition number for a quadratic eigenvalue given in [44]. Figs. 19 and 20 plot the condition number for the quadratic eigenvalue of the notched pillbox with a perfect magnetic and electric boundary condition, respectively. Plotted as a function of $\alpha$, the need for the gauge-fixing coefficient is clear from the singularity in the condition number as $\alpha \to 0$. There is a similar singularity in conditioning at $\alpha = 0$ for the linear system in the driven problem.

The condition number is reasonable for the perfect magnetic boundary condition and there is no strong variation with $\alpha$ or $h_{\text{mesh}}$. The same cannot be said for the impedance or (in the limit of large conductance) perfect electric boundary condition. The addition of the surface integral to impose the perfect electric boundary negatively impacts the condition number. We have found the condition number for a given eigenvalue to scale linearly with the conductance $Y = \frac{1}{Z}$ and as $O(h_{\text{mesh}}^{-2})$ when the impedance boundary is applied. The condition number can be mitigated to some extent by refining the mesh on the boundary while maintaining constant mesh in the interior, but future work will focus on resolving this issue more efficiently by modifying the surface integral or its implementation.

Up to this point, we have focused on specific modes to demonstrate the convergence and stability of the Lagrangian formulation. It is equally important to ensure that in addition to obtaining correct modes, the solved spectrum is free of unphysical modes. Fig. 21(a) plots the spectrum for the first several solved monopole modes of the spherical cavity. Comparing with the theoretically expected modes, we note the presence of two unexpected modes. These are not spurious modes in the conventional sense, however, but rather are pure gauge modes. As can be seen from the mode profiles, these are valid solutions for the four-potential which result in zero field (to within numerical noise). Unlike spurious modes in the nodal curl-curl formulation, these modes converge as the mesh is refined in a similar manner to the expected modes. Most importantly, the number of these pure gauge modes in a given frequency interval does not increase with problem size. In the driven problem, these modes are not excited by sources, as can be seen in Fig. 21(b) (note, only modes with $Az$ on axis are excited so not all resonant modes are present in spectrum). While this example was for a 2-D problem, similar results are obtained in three dimensions, with a proportionally higher number of gauge modes due to the extra dimension.
Fig. 21. Spectrum showing the first several modes of a spherical cavity with 1-m radius as computed through the (a) eigenmode analysis and (b) by scanning the frequency of a driving current and observing the field amplitude. The driven spectrum was excited using a current in the $\hat{z}$ direction, thus, not all resonant modes are reflected in the spectrum. There are two modes in the eigenmode spectrum which are pure gauge modes—valid solutions for the four-potential resulting in vanishing fields. These modes are not excited in the driven problem, as can be seen by the lack of a peak at their respective frequencies. (a) Eigenmode. (b) Driven—relative amplitude of $E_z$ at the origin with an applied current $J_z$ on axis.

Fig. 22. Sample-driven problem where a beam on axis excites the TM$_{011}$ mode of a cylindrical cavity.

D. Charge and Current Density

As discussed in Section III-C, an important feature of the four-potential formulation is the unified framework it provides, accounting for charge and current density independently. This is important in problems where charge conservation is not guaranteed (such as in particle-in-cell codes) or in the low-frequency limit. The following example demonstrates this flexibility and emphasizes the role of the residual gauge freedom in facilitating it. In Fig. 22, a longitudinal current density excites the TM$_{011}$ mode of a cylindrical cavity. This is done by applying a longitudinally varying current density $J_z(\omega, z) = J_0(z - z_c)e^{i\omega t}$ along the cavity axis, where $z_c$ is the $z$-coordinate at the center of the cavity. We can compute the corresponding charge density $\rho$ by applying the charge conservation law to obtain $\rho(\omega, z) = \frac{J_0}{i\omega} z e^{i\omega t}$.

While a conventional field solver is only driven by $\vec{J}$, Fig. 23 shows that in the four-potential formulation, both $\vec{J}$ and $\rho$ drive the solution. Depending on the residual gauge, there are instances where only $\rho$ contributes, when $A_z$ is set to zero everywhere and only $A_r$ and $\phi$ are solved for ($A_\theta$ decouples for $m = 0$ and corresponds only to TE modes so it is not solved for either). Alternatively, $\phi$ can be explicitly set to zero everywhere and the problem is driven entirely by $J_z$. In this case, $\vec{A} \propto \vec{E}$, so in fact this is a conventional nodal field solver and only works because the problem domain is convex. A quantitative comparison of the results is shown in Fig. 24 which plots the integrated absolute value of $E_z$ on axis as a function of driving frequency. The results match to within the expected numerical error in the problem, and agree well with COMSOL, an edge solver only driven by $\vec{J}$.

VI. CONCLUSION

Concluding, we have demonstrated a new FE formulation to solve time harmonic EM fields. By encoding the physics...
of electromagnetism in a different mathematical formulation, the Lagrangian formulation does not suffer from the challenges inherent to the conventional curl-curl equation for \( \vec{E} \). In contrast to the curl-curl equation, where \( \vec{J} \) is the only driving term, our formulation completely accounts for both \( \vec{J} \) and \( \rho \). Both Gauss’ law and Ampere’s law are satisfied, not just globally but over individual elements, in contrast to the commonly employed Nédélec edge elements. This is of importance in the analysis of beam-driven radiation sources, for example, where the contribution to the fields from the space charge \( \rho \), can be significant even at high frequency.

We show through experimental results that the nodal elements are a suitable basis choice for our 4-D formulation. Indeed, our implementation demonstrates that the four-potential formulation easily handles field singularities and discontinuities, unlike nodal element curl-curl implementations. We have benchmarked a proof-of-concept implementation against COMSOL, a state-of-the-art edge element solver, showing that comparable performance can be obtained. Currently, our surface integral for imposing an impedance or perfect electric boundary condition produces accurate results for problem sizes up to around \( n_{\text{DOF}} = 10^5 \). However, the scaling of the condition number with mesh size and conductance needs to be addressed. Finally, we have demonstrated that this approach is not susceptible to spurious modes though pure gauge modes with zero fields do appear in the eigenmode spectrum.

The Lagrangian formulation provides unique opportunities for the numerical analysis of EM fields. While here we present some initial results confirming the accuracy, flexibility, and robustness of this idea, we believe there is much yet to explore, particularly in the time domain. From a practical point of view, the adoption of the four-potential also offers a straightforward solution for those interested in a nodal field solver. This is not only beneficial in terms of the computational efficiency and simplicity of nodal elements, but given the widespread use of nodal elements in fields from structural mechanics to fluid dynamics, allows for a common framework for multiphysics problems.

**APPENDIX**

A. Variation of the Field Theory Lagrangian

The Lagrangian for the EM four-potential including the gauge-fixing term and free sources is given by (17). For simplicity, we assume constant permeability and permittivity, \( \mu \) and \( \epsilon \) in a given mesh element, thus neglecting derivatives of these parameters, however, future work could consider extending this to anisotropic heterogeneous materials even within a mesh element. We also work with \( \alpha = \frac{1}{2} \) as the coefficient of the gauge-fixing term to keep the notation clean. Finally, we are using the metric signature \( (+----) \) in the following:

\[
\mathcal{L} = -\frac{1}{4\mu} F^{\alpha \beta} F_{\alpha \beta} - A_\nu J^\nu - \frac{\alpha}{2} (\partial_\mu A^\mu)^2. \tag{17}
\]

Expanding the four-potential in terms of the components \( A = (\phi, \vec{A}) \) where \( c \) is the speed of light in the medium and, as we working with time harmonic potentials in the frequency domain, replacing derivatives with respect to time by \( i\omega \), we obtain

\[
\mathcal{L} = \frac{1}{2} \left[ (\nabla \phi + i\omega \vec{A}) \cdot (\nabla \phi^* - i\omega \vec{A}^*) - \frac{1}{\mu} (\nabla \times \vec{A}) \cdot (\nabla \times \vec{A}^*) - \frac{\alpha}{\mu} \left( \nabla \cdot \vec{A} + i\omega \frac{\phi}{c^2} \right) \left( \nabla \cdot \vec{A}^* - i\omega \frac{\phi^*}{c^2} \right) - \rho \phi^* - \rho^* \phi + \vec{A} \cdot \vec{J}^* + \vec{A}^* \cdot \vec{J} \right]. \tag{18}
\]

From the point of view of numerical stability and so as to work with parameters having the same dimensions, it is better to normalize \( \phi \) by \( c_0 \), the speed of light in vacuum, and work with \( k_0 = \frac{\omega}{c_0} \) instead of \( \omega \). We thus change to the variable \( \tilde{\phi} = \frac{\phi}{c_0} \). Similarly, for the space charge density, let us define \( \tilde{\rho} = \frac{\rho}{\mu c_0} \).

Finally, let us define a normalized field \( \tilde{E} = \frac{E}{c_0} = -ik_0 \vec{A} - \nabla \tilde{\phi} \). The units of \( \nabla \tilde{\phi} \) and \( k_0 \vec{A} \) are now both \([V]/[s][m]^{-2}\).

This change of variable results in a common factor of \( 2\mu_0 \) over all terms in (18) other than the source terms. We divide the entire expression by this factor and subsequently ignore it as, in the following, we are only interested in setting the variation of this to zero. This gives (19) where \( \epsilon_r \) and \( \mu_r \) are the relative permittivity and permeability. The refractive index \( n = \sqrt{\epsilon_r \mu_r} = c_0/c \) now appears in the gauge-fixing term as we normalized by \( c_0 \) rather than \( c \) (so as to work with the wavenumber in free space).

\[
\mathcal{L} = \epsilon_r (\nabla \tilde{\phi} + ik_0 \vec{A}) \cdot (\nabla \tilde{\phi}^* - ik_0 \vec{A}^*) - \frac{1}{\mu_r} (\nabla \times \vec{A}) \cdot (\nabla \times \vec{A}^*) - \frac{\alpha}{\mu_r} (\nabla \cdot \vec{A} + ik_0 n^2 \tilde{\phi})(\nabla \cdot \vec{A}^* - ik_0 n^2 \tilde{\phi}^*) - \rho \tilde{\phi}^* - \rho^* \tilde{\phi} + \mu_0 \vec{A} \cdot \vec{J}^* + \mu_0 \vec{A}^* \cdot \vec{J}. \tag{19}
\]

The full action integral comprising the variational formulation, including the surface impedance boundary integral, is given in (20). We are interested in taking the variation over the closed volume \( \Omega \) with a perfect magnetic boundary on the surface \( \Gamma_M \) and an impedance boundary on the surface \( \Gamma_Z \). The factor \( \gamma = \frac{1}{\epsilon_r \mu_r c_0} \), the reason for which will be made clear at the end of this appendix.

\[
\mathcal{S} = \int_\Omega \epsilon_r (\nabla \tilde{\phi} + ik_0 \vec{A}) \cdot (\nabla \tilde{\phi}^* - ik_0 \vec{A}^*) - \frac{1}{\mu_r} (\nabla \times \vec{A}) \cdot (\nabla \times \vec{A}^*) - \frac{\alpha}{\mu_r} (\nabla \cdot \vec{A} + ik_0 n^2 \tilde{\phi})(\nabla \cdot \vec{A}^* - ik_0 n^2 \tilde{\phi}^*) - \rho \tilde{\phi}^* - \rho^* \tilde{\phi} + \mu_0 \vec{A} \cdot \vec{J}^* + \mu_0 \vec{A}^* \cdot \vec{J} \ dV + \gamma \int_{\partial \Omega \times} \left( \nabla \times \left( -\nabla \tilde{\phi} - ik_0 \vec{A} \right) \right) \ dS \tag{20}
\]

The variation of (20) with respect to \( \tilde{\phi}^* \) is taken first
\[\delta \phi, S = \int_{\Omega} \epsilon_r \left( \nabla \phi + i k_0 \vec{A} \right) \nabla (\delta \phi^*) - \rho \delta \phi^* \]
\[+ \frac{i k_0 \alpha n^2 \epsilon_r}{\mu_r} \left( \nabla \cdot \vec{A} + i k_0 n^2 \vec{\phi} \right) \delta \phi^* \, dV \]
\[+ \gamma \int_{\Gamma_Z} \left( \hat{n} \times \left( - \nabla \phi - i k_0 \vec{A} \right) \right) \cdot \left( \hat{n} \times \nabla \delta \phi^* \right) \, dS \]
\[= \epsilon_r \int_{\Omega} \left( i k_0 (\alpha - 1) \nabla \cdot \vec{A} - \alpha n^2 k_0^2 \vec{\phi} - \nabla^2 \phi - \frac{\rho}{\epsilon_r} \right) \delta \phi^* \, dV \]
\[+ \epsilon_r \int_{\partial \Omega} \left( \nabla \phi + i k_0 \vec{A} \right) \delta \phi^* \, dS + \gamma \int_{\Gamma_Z} \left[ \left( - \nabla \phi - i k_0 \vec{A} \right) \hat{n} \right] \nabla (\delta \phi^*) \, dS \]  
\[(21)\]

where we applied the divergence theorem and the identity \((\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = (\vec{A} \cdot \vec{C}) (\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D}) (\vec{B} \cdot \vec{C})\) to the impedance integral. Let us define the projection of \(\vec{E}\) on the tangent surface as \(\vec{E}_t = \vec{E} - (\vec{E} \cdot \hat{n}) \hat{n}\) (note that this is orthogonal to \(\hat{n} \times \vec{E}\)). Next, we apply the vector identity, \(\vec{B} \cdot \nabla \alpha = \nabla \cdot (\alpha \vec{B}) - \alpha \nabla \cdot \vec{B}\) to the impedance surface integral

\[\delta \phi, S = \epsilon_r \int_{\Omega} \left( i k_0 (\alpha - 1) \nabla \cdot \vec{A} - \alpha n^2 k_0^2 \vec{\phi} \right) \]
\[\quad - \nabla^2 \phi - \frac{\rho}{\epsilon_r} \, dV \]
\[+ \epsilon_r \int_{\partial \Omega} \left( \nabla \phi + i k_0 \vec{A} \right) \delta \phi^* \, dS + \gamma \int_{\Gamma_Z} \left( \vec{E}_t \delta \phi^* \right) - \nabla \cdot (\vec{E}_t) \delta \phi^* \, dS. \]  
\[(22)\]

We can then apply the divergence theorem on a surface to convert the first term in the impedance boundary to a line integral which vanishes over a closed surface. The corresponding set of equations enforced through the variation with respect to \(\phi^*\) is then given by (24)–(26) where we have given the final system of equations in terms of the unnormalized potential and fields. There is also a corresponding set for the complex conjugate terms, obtained through the variation with respect to \(\phi\).

\[\alpha n^2 k_0^2 \phi + \nabla^2 \phi - i k_0 (\alpha - 1) \nabla \cdot \vec{A} = -\frac{\rho}{\epsilon} \] in \(\Omega\)  
\[(24)\]
\[\left( - \nabla \phi - ik_0 \vec{A} \right) \cdot \hat{n} = E_n = 0 \text{ on } \Gamma_{PM}\]  
\[(25)\]
\[\epsilon_r E_n + \gamma \nabla \cdot \vec{E}_t = 0 \text{ on } \Gamma_Z\]  
\[(26)\]

We shall reserve the discussion of these terms until after the variation with respect to \(\vec{A}^*\), which we now take

\[\delta \vec{A}, S = \int_{\Omega} \left[ - i k_0 \epsilon_r (\nabla \phi + i k_0 \vec{A}) \delta \vec{A}^* + \mu_0 \vec{J} \cdot \delta \vec{A}^* \right. \]
\[\quad - \frac{\alpha}{\mu_r} (\nabla \cdot \vec{A} + i k_0 n^2 \vec{\phi}) \nabla \cdot \delta \vec{A}^* \]
\[\left. - \frac{1}{\mu_r} (\nabla \times \vec{A}) \cdot (\nabla \times \delta \vec{A}^*) \right) \, dV \]
\[+ i k_0 \gamma \int_{\Gamma_Z} \left[ \hat{n} \times (- \nabla \phi - i k_0 \vec{A}) \right] \cdot (\hat{n} \times \delta \vec{A}^*) \, dS \]  
\[(27)\]

\[= \int_{\Omega} \left[ - i k_0 \epsilon_r \nabla \phi + \epsilon_r k_0^2 \vec{A} + \mu_0 \vec{J} + \frac{\alpha}{\mu_r} (\nabla \cdot \vec{A} + i k_0 n^2 \vec{\phi}) \right. \]
\[\quad - \frac{1}{\mu_r} \nabla \times (\nabla \times \vec{A}) \right] \cdot \delta \vec{A}^* \, dV \]
\[\quad - \frac{1}{\mu_r} \int_{\partial \Omega} \left( \delta \vec{A}^* \times (\nabla \times \vec{A}) \right) \cdot \hat{n} \, dS \]
\[+ i k_0 \gamma \int_{\Gamma_Z} \left[ (- \nabla \phi - i k_0 \vec{A}) - \left( (- \nabla \phi - i k_0 \vec{A}) \cdot \hat{n} \right) \hat{n} \right] \cdot \delta \vec{A}^* \, dS \]  
\[(28)\]

The total set of equations that are satisfied when \(S\) is minimized (including (24)–(26) obtained through the variation with respect to \(\phi^*\) are as follows. Once again, we have substituted the original expressions for \(\phi, \vec{E}\), and \(\rho\) into these equations

\[\alpha n^2 k_0^2 \phi + \nabla^2 \phi - i k_0 (\alpha - 1) \nabla \cdot \vec{A} = -\frac{\rho}{\epsilon} \] in \(\Omega\)  
\[(30)\]
\[\left( - \nabla \phi - ik_0 \vec{A} \right) \hat{n} = E_n = 0 \text{ on } \Gamma_{PM}\]  
\[(31)\]
\[\hat{n} \times (\nabla \times \vec{A}) - \alpha (\nabla \cdot \vec{A} + i \omega \epsilon^{-1} \phi) \hat{n} = 0 \text{ on } \Gamma_{PM}\]  
\[(32)\]
\[\epsilon_r E_n + \gamma \nabla \cdot \vec{E}_t = 0 \text{ on } \Gamma_Z\]  
\[(33)\]
\[\hat{n} \times (\nabla \times \vec{A}) - \alpha (\nabla \cdot \vec{A} + i \omega \epsilon^{-1} \phi) \hat{n} + \frac{i k_0 \mu_0 \gamma}{\epsilon_0} \vec{E}_t = 0 \text{ on } \Gamma_Z.\]  
\[(34)\]

Once again, there is another set of equations consisting of the complex conjugate terms, corresponding to the variation with respect to \(\phi\) and \(\vec{A}\). When the Lorenz gauge is enforced, \(\nabla \cdot \vec{A} + i \omega \phi = 0\) and the boundary conditions imposed by the natural boundary condition are those corresponding to a perfect magnetic conductor

\[\vec{E}_n = 0\]  
\[(36)\]
\[\hat{n} \times (\nabla \times \vec{A}) = \hat{n} \times \vec{B} = \vec{B}_t = 0.\]  
\[(37)\]

Meanwhile, on the surface with the impedance surface integral added \(\Gamma_Z\), the boundary condition imposed by the variation
with $\tilde{A}$ is as follows:

$$
\tilde{E}_t = \tilde{E} - (\tilde{E} \cdot \hat{n})\hat{n} = -\frac{c_0}{ik_0 \gamma \mu_r} \tilde{B}_t = -\frac{c_0 \mu_0}{ik_0 \gamma} \tilde{H}_t = Z \tilde{H}_t
$$

(38)

from which we determine the relationship between our original $\gamma$ and the complex impedance on the boundary $Z$

$$
\gamma = -\frac{c_0 \mu_0}{ik_0 Z} = -\frac{1}{i \epsilon \omega Z}.
$$

(39)

B. Splitting of the Lagrangian for $\alpha = 1$

If the coefficient for the gauge-fixing term is equal to one, there is a splitting of the Lagrangian within the volume

$$
\mathcal{L} = \frac{1}{2} \left[ (\nabla \phi + i \omega \tilde{A}) \cdot (\nabla \phi^* - i \omega \tilde{A}) - \frac{1}{\mu} (\nabla \times \tilde{A}) \cdot (\nabla \times \tilde{A}^*) - \frac{1}{\mu_c} \left( \nabla \cdot \tilde{A} + i \frac{\omega}{c^2} \phi \right) \left( \nabla \cdot \tilde{A}^* - i \frac{\omega}{c^2} \phi^* \right) - \rho \phi^* - \rho^* \phi + \tilde{A} \cdot J + \tilde{A}^* \cdot J \right]
$$

$$
\mathcal{L} = \frac{1}{2} \left[ \frac{\epsilon_r}{2} \int_{\Omega} \left( |\nabla \phi|^2 + \omega^2 |\tilde{A}|^2 - \frac{\omega^2}{c^2} |\phi|^2 \right) - \frac{1}{\mu} \left( |\nabla \times \tilde{A}|^2 + |\nabla \cdot \tilde{A}|^2 \right) + i \omega \left( \phi \cdot \nabla \cdot \tilde{A} - \nabla \cdot \tilde{A}^* \phi + \tilde{A} \cdot \nabla \phi^* - \tilde{A}^* \cdot \nabla \phi \right) \right]
$$

$$
- \rho \phi^* - \rho^* \phi + \tilde{A} \cdot J + \tilde{A}^* \cdot J.
$$

(40)

Applying the same transformation as between (18) and (19) results in the following:

$$
\mathcal{L} = \epsilon_r \left( |\nabla \phi|^2 + \frac{k_0^2}{\epsilon} |\tilde{A}|^2 - k_0^2 |\phi|^2 \right)
$$

$$
- \frac{1}{\mu_c} \left( |\nabla \times \tilde{A}|^2 + |\nabla \cdot \tilde{A}|^2 \right) + ik_0 \mu_r \epsilon_r \left( \phi \cdot \nabla \cdot \tilde{A} - \nabla \cdot \tilde{A}^* \phi + \tilde{A} \cdot \nabla \phi^* - \tilde{A}^* \cdot \nabla \phi \right)
$$

$$
- \rho \phi^* - \rho^* \phi + \tilde{A} \cdot J + \tilde{A}^* \cdot J.
$$

(41)

Integrating $\mathcal{L}$ over the volume to obtain the action integral, we find that the coupling terms between $\tilde{A}$ and $\tilde{\phi}$ can be written purely in terms of surface integrals. This is accomplished through the identity: $\int_{\Omega} \phi^* \nabla \cdot \tilde{A} \ dV = \int_{\partial \Omega} \phi^* \tilde{A} \cdot \hat{n} \ dS - \int_{\Omega} \nabla \phi^* \cdot \tilde{A} \ dV$

$$
S = \int_{\Omega} \mathcal{L} \ dV = \int_{\Omega} \int_{\partial \Omega} \phi^* \tilde{A} \cdot \hat{n} \ dS - \int_{\Omega} \nabla \phi^* \cdot \tilde{A} \ dV
$$

$$
S = \int_{\Omega} \int_{\partial \Omega} \phi^* \tilde{A} \cdot \hat{n} \ dS - \int_{\Omega} \nabla \phi^* \cdot \tilde{A} \ dV
$$

The scalar components of $\tilde{A}$ also split within the volume. Noting that $\int_{\Omega} \nabla \cdot \tilde{A}^* (\nabla \cdot \tilde{A}) \ dV = \int_{\partial \Omega} (\nabla \cdot \tilde{A}^*) \tilde{A} \cdot \hat{n} \ dS$

$$
\int_{\Omega} \nabla \cdot \tilde{A}^* \cdot \tilde{A} \ dV
$$

and using the identity, $\nabla \cdot (\tilde{u} \times \tilde{v}) = \tilde{v} \cdot (\nabla \times \tilde{u}) - \tilde{u} \cdot (\nabla \times \tilde{v})$ to obtain $\int_{\Omega} \nabla \cdot \tilde{A}^* \cdot (\nabla \times \tilde{A}) \ dV = \int_{\Omega} \nabla \cdot (\tilde{A} \times (\nabla \times \tilde{A}^*) + (\nabla \times (\nabla \times \tilde{A}^*)) \ dV$, we obtain (43). Note also the use of the vector Laplacian $\nabla^2 \tilde{A}^* = \nabla (\nabla \cdot \tilde{A}^*) - \nabla \times (\nabla \times \tilde{A}^*) = (\nabla^2 A_x, \nabla^2 A_y, \nabla^2 A_z)$

$$
S = S_\phi + S_{A_x} + S_{A_y} + S_{A_z} + S_c
$$

(43)

where the first four terms are computed within the volume (cacc stands for the complex conjugate terms), with $i \in (x, y, z)$ as follows:

$$
S_\phi = \int_{\Omega} \int_{\partial \Omega} \left( |\nabla \tilde{\phi}|^2 + |\phi|^2 \right) - \rho \tilde{\phi}^* - \rho^* \tilde{\phi} \ dV
$$

$$
S_{A_x} = \int_{\Omega} \int_{\partial \Omega} \left( |\nabla \phi|^2 + |\phi|^2 \right)
$$

$$
\times (\nabla \times \tilde{A}^*) \cdot \hat{n} \ dS + c.c.
$$

(46)

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