A Generalized Tree-Cotree Gauge for Magnetic Field Computation

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***Abstract* -- The discretization of the magnetostatic curl-curl equation using edge-based elements results in a singular matrix equation. As has been shown previously, this matrix may be made nonsingular by eliminating the matrix nullspace. A generalization of this process is presented in this paper that does not require setting field quantities to zero, thus allowing the gauge in vector potential solutions to be set in a more natural way. This process also makes it possible to solve for the electric or magnetic field directly in high frequency applications.**

I. INTRODUCTION

Electromagnetic field computation by the finite element method often involves the discretization of the curl-curl operator. Magnetostatic problems solved in terms of the vector potential $\vec{A}$ are described by setting the curl-curl of $\vec{A}$ equal to the permeability times the current density, while high frequency problems are often solved directly for the electric or magnetic field by computing the eigenvalues and eigenvectors of the curl-curl operator. Early work in this area used standard scalar finite elements for this purpose and generated numerical instabilities called spurious modes with high frequency problems [1] and mesh-dependent solutions with magnetostatic problems [2]. More recent work has employed edge-based vector finite elements in which the solution variables represent the tangential components of the field variable along the edges of the finite element. It has been shown that tangential vector finite elements eliminate the problem of spurious modes and of mesh-dependent solutions [3]. It has been shown further that tangential elements work correctly because the curl-curl operator has a non-trivial nullspace and these elements approximate the nullspace of the curl-curl operator properly [3].

Since tangential finite elements approximate the nullspace of the curl-curl operator properly, discretizing this operator using these elements results in singular matrices. While the answers produced by these elements are correct, the resulting singular matrices encountered in magnetostatic, eddy current, and high frequency scattering problems, exhibit poor and unreliable convergence if the equations are solved with the conjugate gradient method. In eigenvalue solutions such as encountered in cavity resonance and waveguide problems, the curl-curl matrix singularity results in unwanted zero eigenvalues and corresponding eigenvectors.

This paper builds on the work of Albanese and Rubinacci for eliminating the nullspace of the matrix formed by approximating the curl-curl operator using tangential vector finite elements [4]. They showed that one may convert the singular matrices obtained with edge-based solutions of magnetostatic problems into nonsingular matrices by setting the vector potential on the tree of the graph of the finite element mesh to zero.

This paper presents a general procedure for eliminating the nullspace of the curl-curl matrix. We show that the finite element curl-curl matrix is partitioned naturally into two orthogonal subspaces by the tree and cotree of the graph of the finite element mesh used to generate it. We derive procedures for computing the relationships between these subspaces, and for computing solutions in general. Finally, we show both theoretically and by numerical examples that a generalized tree-cotree gauge may be used to compute magnetic vector potentials and to eliminate unwanted zero eigenvalues in high-frequency problems.

II. MAGNETOSTATICS

Consider a two or three dimensional problem domain Ω with boundary S and prescribed current density $\vec{J}$. The magnetostatic field may be determined in Ω by solving the differential equation

$$\nabla \times \frac{1}{\mu} \nabla \times \vec{A} = \vec{J} \tag{1}$$

where $\vec{A}$ is the vector potential. For simplicity and without reducing the generality of the following analysis, we assume a magnetic wall boundary condition on the whole of S:

$$\hat{n} \times \frac{1}{\mu} \nabla \times \vec{A} = \mathbf{0} \ . \tag{2}$$

Since the divergence of $\vec{A}$ is not specified by (1) and (2), any solution $\vec{A}$ to these equations has the property that $\vec{A} + \nabla\phi$ is also a solution. Thus, the curl-curl operator has a non-trivial nullspace which includes the gradient of any differentiable scalar function ϕ. Additionally note that $\vec{J}$ cannot be specified arbitrarily because (1) requires $\nabla \cdot \vec{J} = 0$.

Manuscript received July 5, 1994; revised Nov 22, 1994.

0018-9464/95$04.00

The variational principle used to solve (1) and (2) with the finite element method is generated by the functional

$$F(\vec{\mathbf{A}}') = \frac{1}{2}\int_{\Omega} \frac{1}{\mu}|\nabla \times \vec{\mathbf{A}}'|^2 dV - \int_{\Omega} \vec{\mathbf{J}} \cdot \vec{\mathbf{A}}' dV \ . \quad (3)$$

Minimizing $F(\vec{\mathbf{A}}')$ over the space of finite elements results in an approximate solution for the vector potential $\vec{\mathbf{A}}$. Let zero order tangential finite element basis functions be denoted by $\vec{\mathbf{e}}_i$, $i = 1, ..., E$ where E is the number of edges in the finite element mesh [5]. Minimization of $F(\vec{\mathbf{A}}')$ then results in the following matrix equation for the $E{\times}1$ unknown column vector $\mathbf{A}$

$$[S]\,\mathbf{A} = \mathbf{b} \quad (4)$$

where the $E{\times}E$ matrix [S] and the $E{\times}1$ column vector $\mathbf{b}$ are defined by

$$S_{ij} = \int_{\Omega} \frac{1}{\mu}\nabla \times \vec{\mathbf{e}}_i \cdot \nabla \times \vec{\mathbf{e}}_j \, dV \quad (5)$$

and

$$b_i = \int_{\Omega} \vec{\mathbf{J}} \cdot \vec{\mathbf{e}}_i \, dV \quad (6)$$

respectively. The matrix $[S]$ (the "curl-curl matrix") is singular and thus mimics the singularity of the continuous problem. Analogous to the continuous problem (1) and (2), the singularity of $[S]$ raises two issues. First, what are the requirements on $\mathbf{b}$ so that $\mathbf{b}$ is in the range of $[S]$? Second, how should the domain of $[S]$ be restricted to yield a numerical solution to (4)?

III. THE STRUCTURE OF THE CURL-CURL MATRIX

Following Albanese and Rubinacci [4], we relate the structure of $[S]$ to the properties of the graph of the finite element mesh. We do this in two steps: First we show that $[S]$ is row equivalent to the matrix $[C]$ representing the curl operator. Then we establish a relationship between $[C]$ and the mesh, thereby defining a relationship between $[S]$ and the mesh.

A. Row equivalence of [S] and [C]

To accomplish the first step we characterize the nullspace of $[S]$. This is defined as solutions $\mathbf{A}$ to the equation

$$[S]\mathbf{A} = \mathbf{0} \quad (7)$$

The variational principle (3) implies that

$$[S]\mathbf{A} = 0 \Leftrightarrow minimize\ F(\vec{\mathbf{A}}') = \quad (8)$$

$$\int_{\Omega} \frac{1}{\mu}|\nabla \times \vec{\mathbf{A}}'|^2 dV = \sum_{i=1}^{T} \int_{\Delta_i} \frac{1}{\mu}|\nabla \times \vec{\mathbf{A}}'|^2 dV$$

where T = the number of elements, $\vec{\mathbf{A}}'$ is the vector field generated by multiplying the basis functions $\vec{\mathbf{e}}_i$ by the components of $\mathbf{A}'$, and Δ_i denotes the i-th element. Since $|\nabla{\times}\vec{\mathbf{A}}'|^2 \geq 0$, (8) is equivalent to $\nabla{\times}\vec{\mathbf{A}}' = \mathbf{0}$ in each element Δ_i. $\nabla{\times}\vec{\mathbf{A}}' = \mathbf{0}$ is represented by the matrix equation

$$[C]\mathbf{A} = \mathbf{0} \quad (9)$$

where the matrix $[C]$ is a T×E matrix if Ω is 2D and 3T×E matrix if Ω is 3D. Here each row of $[C]$ contains exactly three nonzero entries which select the proper linear combination of edge variables to compute a component of the curl of the field described by $\mathbf{A}$ within the corresponding element. Since $[S]\mathbf{A} = \mathbf{0} \Rightarrow [C]\mathbf{A} = \mathbf{0}$, $[S]$ and $[C]$ share the same nullspace and therefore are row equivalent.

B. Relation of [C] to the finite element mesh

Albanese and Rubinacci show that the set of edges formed by any cotree of a finite element mesh provides a set of linearly independent degrees of freedom for representing the curl operator. The corresponding set of edges that may be set arbitrarily is described by the corresponding tree [4]. Now consider the same process of setting $\nabla{\times}\vec{\mathbf{A}}$ in terms of the $[C]$ matrix. The process is represented algebraically as $[C]\mathbf{A} = \mathbf{B}$ where $\mathbf{B}$ is a column vector containing the desired curl values for each element. Since $[C]$ has more columns than rows, applying the Gaussian elimination algorithm with full pivoting provides components of $\mathbf{A}$ corresponding to the pivots that establish the solution while the remainder are arbitrary [6]. We will call the variables corresponding to the pivots the "pivot variables" and the others the "free variables".

As noted previously, these same properties define the tree and cotree edges of a finite element mesh. Therefore identifying the free variables and the pivot variables for $[C]$ is possible by simple inspection of the mesh. Also since $[S]$ is row equivalent to $[C]$, in equation (4) $[S]$ may be partitioned as follows

$$\begin{bmatrix} S_{CC} & S_{CT} \\ S_{TC} & S_{TT} \end{bmatrix} \begin{bmatrix} \mathbf{A}_C \\ \mathbf{A}_T \end{bmatrix} = \begin{bmatrix} \mathbf{b}_C \\ \mathbf{b}_T \end{bmatrix} \quad (10)$$

In this equation, the edges corresponding to the cotree are numbered first, the edges corresponding to the tree are numbered second, and subscripts "C" and "T" stand for cotree and tree respectively. The $C{\times}C$ submatrix S_{CC} is symmetric positive definite.

IV. SINGULAR MATRIX EQUATION SOLUTION

Using the above partitioned form for $[S]$, we answer the two questions posed at the end of the introduction. In what follows range$[S]$ is the set $\{\mathbf{b} \in R^E | [S]\mathbf{x} = \mathbf{b}$ for some $\mathbf{x} \in R^E\}$, $N[S]$ denotes the nullspace of $[S] = \{\mathbf{x} \in R^E | [S]\mathbf{x} = \mathbf{0}\}$, and $N^{\perp}[S] = \{\mathbf{x} \in R^E | \langle\mathbf{x},\mathbf{y}\rangle = 0$ for all $\mathbf{y} \in N[S]\}$. Here R^E is the space of E-dimensional column vectors and $\langle\mathbf{x},\mathbf{y}\rangle$ is the usual Euclidean inner product of two column vectors $\mathbf{x},\mathbf{y}$.

A. Requirements on b for a solution to exist

To derive a necessary condition for $\mathbf{b} \in$ range$[S]$ we note the following. For $\mathbf{y} \in N[S]$ we have $[S]\mathbf{y} = \mathbf{0}$ and so taking inner products of both sides of (4):

$$\langle \mathbf{b},\mathbf{y}\rangle = \langle [S]\mathbf{A},\mathbf{y}\rangle = \langle \mathbf{A},[S]\mathbf{y}\rangle = 0 \qquad (11)$$

where symmetry of $[S]$ has been used. Therefore $\mathbf{b}$ must be perpendicular to the entire nullspace of $[S]$, i.e. $\mathbf{b} \in N^{\perp}[S]$. Now $\mathbf{b} \in N^{\perp}[S]$ implies $\mathbf{b}$ is a linear combination of rows of $[S]$ (true for any matrix [6]) so $\mathbf{b} = [S]^T\mathbf{z}$ for some $\mathbf{z} \in R^E$ where the superscript "T" denotes matrix transpose. Written in partitioned matrix form:

$$\begin{bmatrix} \mathbf{b}_C \\ \mathbf{b}_T \end{bmatrix} = \begin{bmatrix} S_{CC} & S_{CT} \\ S_{TC} & S_{TT} \end{bmatrix} \begin{bmatrix} \mathbf{z}_C \\ \mathbf{z}_T \end{bmatrix} \qquad (12)$$

This yields the two equations

$$S_{CC}^{-1}\,\mathbf{b}_C = \mathbf{z}_C + S_{CC}^{-1}\,S_{CT}\,\mathbf{z}_T \qquad (13)$$

$$\mathbf{b}_T = S_{TC}\,\mathbf{z}_C + S_{TT}\,\mathbf{z}_T \qquad (14)$$

Eliminating $\mathbf{z}_C$ and using the $[S]$ matrix relation $S_{TT} = S_{TC}S_{CC}^{-1}S_{CT}$ (easily shown), we obtain the following relation between the portions of $\mathbf{b}$:

$$\mathbf{b}_T = S_{TC}S_{CC}^{-1}\mathbf{b}_C \qquad (15)$$

This is an algebraic constraint on $\mathbf{b}$ so that $[S]\mathbf{A} = \mathbf{b}$ will have a solution. It can in principle be used to verify that a computed $\mathbf{b}$ is in the range of $[S]$ prior to solution of (4). However a more meaningful interpretation arises from consideration of the field defined by $\vec{J}_p = \mathbf{b}^T\mathbf{e}$ (the projection of the current density field $\vec{J}$ onto the edge element space). Here $\mathbf{e}$ is the $Ex1$ column vector of edge element basis functions. The significance of $\vec{J}_p$ is discussed in section VIII.

B. Generating Solutions to $[S]\mathbf{A} = \mathbf{b}$

Given that $\mathbf{b}$ satisfies the condition (15), all solutions to $[S]\mathbf{A} = \mathbf{b}$ can be expressed using the submatrices of $[S]$. Writing the matrix equation (4) as

$$\begin{bmatrix} S_{CC}\mathbf{A}_C + S_{CT}\mathbf{A}_T \\ S_{TC}\mathbf{A}_C + S_{TT}\mathbf{A}_T \end{bmatrix} = \begin{bmatrix} \mathbf{b}_C \\ \mathbf{b}_T \end{bmatrix} \qquad (16)$$

the first row can be solved for $\mathbf{A}_C$

$$\mathbf{A}_C = S_{CC}^{-1}(\mathbf{b}_C - S_{CT}\mathbf{A}_T) \qquad (17)$$

Making any choice for $\mathbf{A}_T$ we can show the second row of (16) is automatically satisfied. To do this multiply (17) by S_{TC} and rearrange to obtain

$$S_{TC}\mathbf{A}_C + S_{TC}S_{CC}^{-1}S_{CT}\mathbf{A}_T = S_{TC}S_{CC}^{-1}\mathbf{b}_C \qquad (18)$$

Then using $S_{TT} = S_{TC}S_{CC}^{-1}S_{CT}$ and (15), (18) becomes

$$S_{TC}\mathbf{A}_C + S_{TT}\mathbf{A}_T = \mathbf{b}_T \qquad (19)$$

which is the second row of (16).

To summarize, the infinite family of solutions to $[S]\mathbf{A}=\mathbf{b}$ is generated by arbitrarily setting values on the mesh tree $\mathbf{A}_T$ and solving

$$S_{CC}\mathbf{A}_C = \mathbf{b}_C - S_{CT}\mathbf{A}_T \qquad (20)$$

for $\mathbf{A}_C$.

C. Reduction in problem order

Since S_{CC} is CxC, (20) represents a reduction in order of the original ExE square system from E to C. To quantitatively evaluate this decrease we note that $C = E - B$ where B is the number of branches in the tree. Now let N denote the number of nodes in the mesh. Then it can be shown that [7]

$$B = N - 1\,. \qquad (21)$$

Using this fact, $C = E - N + 1$. Now for large meshes in 2D, $E/N \rightarrow 3$ [7] and in this case reduction in order from E to C represents a 33% decrease. For large 3D meshes generated using Delaunay tessellation a good approximation is $E/N = 7.3$ [8] with a corresponding 14% decrease in problem order.

V. THE ZERO TREE GAUGE

The simplest choice for $\mathbf{A}_T$ in (20) is $\mathbf{A}_T = \mathbf{0}$ [2]. The solution domain is thereby reduced to the cotree edges and the following CxC positive definite system results

$$S_{CC}\mathbf{A}_C = \mathbf{b}_C \qquad (22)$$

To illustrate, consider the 2-dimensional problem pictured in Fig. 1 consisting of a square solenoid in which an impressed current density $\vec{\mathbf{J}}$ circulates around an iron core with $\mu_r = 5.0$. The magnetic vector potential obeys (1) within the problem domain. The flux is confined to the problem domain by the natural boundary condition of the functional. Fig. 2 depicts a finite element mesh (N = 142, T = 249, E = 390) for the problem region in Fig. 1. Fig. 3 is a tree of the Fig. 2 mesh with 141 branches. The corresponding cotree therefore has 390 − 141 = 249 edges. The vector field $\vec{\mathbf{A}}$ derived from solving (4) in which edge variables are set to zero on the tree branches is shown in Fig. 4. The resulting field $\vec{\mathbf{B}} = \nabla \times \vec{\mathbf{A}}$ in Fig. 5 is uniform across the magnetic material and decays to zero at the magnetic wall boundary.

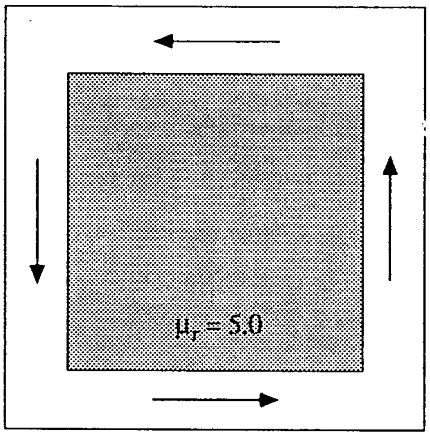

Fig. 1. Square iron core solenoid

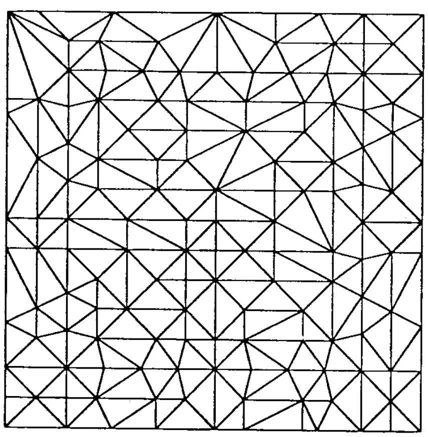

Fig. 2. A Finite element mesh for the square solenoid

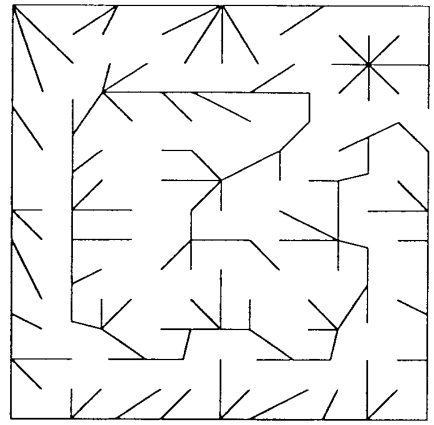

Fig. 3. A tree for the mesh in Fig. 2

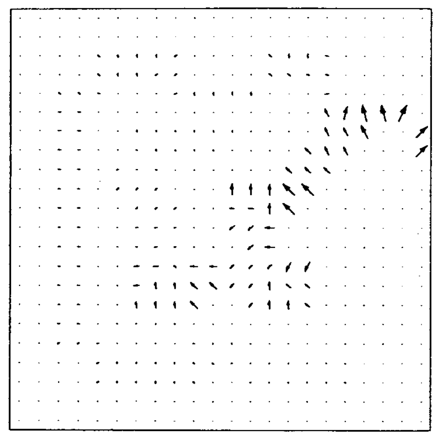

Fig. 4. Zero tree gauge vector potential $\vec{\mathbf{A}}$

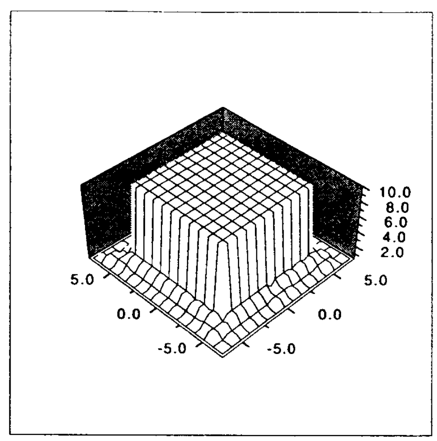

Fig. 5. Magnetic flux density obtained by taking the curl of $\vec{\mathbf{A}}$ in Fig. 4

VI. THE COULOMB GAUGE

In the preceding analysis, the vector potential is set arbitrarily to zero on the mesh tree without affecting the corresponding field $\vec{\mathbf{B}} = \nabla \times \vec{\mathbf{A}}$. We now consider the possibility of gauging $\vec{\mathbf{A}}$ without arbitrarily setting certain values to zero. Since the nontrivial $[S]$ nullspace is the cause of the matrix singularity, we restrict the solution domain to be orthogonal to this nullspace. Since the nullspace of a matrix is the orthogonal complement of the rowspace in R^E we restrict the solution to be a linear combination of the rows of $[S]$. This is accomplished by the formal change of variable from $\mathbf{A}$ to $\mathbf{y}$ defined by

$$\mathbf{A} = [H]^T \mathbf{y} \tag{23}$$

where $\mathbf{y}$ is a $C \times 1$ vector and the $C \times E$ matrix $[H]$ consists of the upper C rows of the reordered $[S]$-matrix.

$$[H] \equiv [\, S_{CC} \vdots S_{CT} \,] \tag{24}$$

Using (23) in (4) and performing the multiplication gives the system

$$[H][H]^T \mathbf{y} = \mathbf{b}_C \tag{25}$$

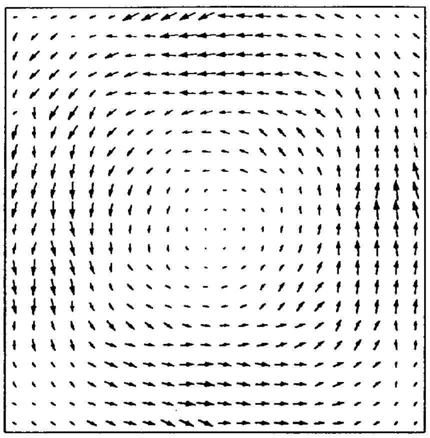

Fig. 6. Vector potential $\vec{\mathbf{A}}_0$ computed using equation (23)

The $C \times C$ matrix $[H][H]^T$ is symmetric and positive definite. Solving (25) yields $\mathbf{y}$; (23) then gives $\mathbf{A}$. Fig. 6 depicts the solution of (1) and (2) in the problem domain of Fig. 1 using the mesh and tree of Fig. 2 and Fig. 3. Here the nullspace gauge was enforced by (23) to give (25). The resulting vector potential, denoted $\vec{\mathbf{A}}_0$, lacks the abrupt jumps in normal component across element boundaries exhibited by the zero tree gauge in Fig. 4. Section VIII discusses how this behavior relates $\vec{\mathbf{A}}_0$ to the magnetostatic Coulomb gauge. Evaluating the curl of $\vec{\mathbf{A}}_0$ in Fig. 6 to give $\vec{\mathbf{B}}$ yields the identical magnetic flux density computed from $\vec{\mathbf{A}}$ in Fig. 4 and shown in Fig. 5.

Despite the more "natural" appearance of the nullspace gauge vector potential, the system (25) is in general less sparse than the zero-tree gauge system (22) and numerical experiments have not yet shown computational advantage of (25) over (22).

VII. EIGENVALUE PROBLEMS

Eigenvalue problems arise in the context of finite element solutions to cavity resonators and waveguides and have the feature that the solution variable is usually the field itself, $\vec{\mathbf{E}}$ or $\vec{\mathbf{H}}$, rather than a potential function. Using edge elements to approximate the field models the nullspace of the curl-curl operator correctly and results in zero eigenvalues. The question is: Is it possible to reduce the size of the matrix eigenvalue problem by eliminating these zero eigenvalues? The fact that the source of the zero eigenvalue solutions is again the nullspace of the $[S]$-matrix suggests that the transformation (23) may be used again in eliminating these unwanted solutions.

A. Solution of the vector wave equation

Consider the matrix eigenvalue problem

$$[S]\mathbf{x} = \lambda[T]\mathbf{x} \tag{26}$$

resulting from discretization of the time-harmonic vector wave equation for $\vec{\mathbf{E}}$

$$\nabla \times \frac{1}{\mu_r} \nabla \times \vec{\mathbf{E}} = \varepsilon_r k_0^2 \vec{\mathbf{E}} \tag{27}$$

or its dual form for $\vec{\mathbf{H}}$, on a mesh with E edges where $[S]$ is defined as before and $[T]$ is the positive definite $E \times E$ matrix

$$T_{ij} = \int_\Omega \mu_r \, \vec{\mathbf{e}}_i \cdot \vec{\mathbf{e}}_j \, dV \ . \tag{28}$$

The eigenvectors corresponding to the zero eigenvalues of (26) span the nullspace of $[S]$ since when $[S]\mathbf{y} = \mathbf{0}$, $[S]\mathbf{y} = \lambda[T]\mathbf{y}$ with $\lambda = 0$. To eliminate the nullspace we employ the fact that the eigenvectors of a general, real, symmetric matrix corresponding to different eigenvalues are $[T]$-orthogonal [6]:

$$\mathbf{x}_i^T [T] \, \mathbf{x}_j = \mathbf{0} \quad \textit{if } i \neq j. \tag{29}$$

Analogous to (23) set

$$\mathbf{x} = [T]^{-1} [H]^T \mathbf{y} \ . \tag{30}$$

Note that for $x_0 \in N[S]$ and $\mathbf{x}$ computed from (30):

$$\mathbf{x}_0^T[T]\mathbf{x} = \mathbf{x}_0^T[T][T]^{-1}[H]^T\mathbf{y} = \mathbf{x}_0^T[H]^T\mathbf{y} = 0 \ . \quad (31)$$

The new system

$$[S']y = \lambda[T']y \quad (32)$$

where

$$[S'] = \left([H][T]^{-1}\right)[S]\left([H][T]^{-1}\right)^T \quad (33)$$

$$[T'] = \left([H][T]^{-1}\right)[T]\left([H][T]^{-1}\right)^T \quad (34)$$

are $C \times C$ matrices, excludes the nullspace and hence the zero eigenvalues while preserving the non-zero eigenvalues from the original $E \times E$ system (26). Numerical experiments involving the solution of the vector wave equation (27) in rectangular cavities and uniform cross section waveguides have confirmed the formulation (32).

B. Essential boundary conditions

In the solution of cavity and waveguide problems it is desirable to use $\vec{\mathbf{E}}$ as a solution variable and enforce homogeneous Dirichlet boundary conditions on the structure walls to reduce the order of the final eigenvalue problem. In this case edges on the boundary are fixed so construction of a mesh tree initially takes place on the N_{int} interior nodes giving $N_{int} - 1$ edges in accord with the general result (21). One additional edge extending to the boundary may be included without forming any closed loops giving the final result $B = N_{int} - 1 + 1 = N_{int}$. By its partitioned structure (10), $[S]$ has $B = N_{int}$ dependent rows and therefore the problem (26) has N_{int} zero eigenvalues. This expression for the number of zero eigenvalues has been noted empirically before [9] and also derived using nodal elements in a joint vector and scalar potential formulation [10].

VIII. NORMAL CONTINUITY

Equation (27) supports two classes of solutions corresponding to zero and non-zero eigenvalues. In the former case $\nabla \cdot \varepsilon \vec{\mathbf{E}} = 0$; in the latter $\nabla \cdot \varepsilon \vec{\mathbf{E}} \neq 0$ in general. By eliminating the zero eigenvalue solutions the transformation (30) represents a restriction of the discrete problem domain to weak-sense normally continuous fields.

In the magnetostatic case, equivalent transformations establish the nullspace gauge via (23) and also define vectors $\mathbf{b}$ in range$[S]$ via (12). It is conjectured on the basis of computed results such as Fig. 6 and similarity to (30), that (23) and (12) establish weak-sense normal continuity of the fields $\vec{\mathbf{A}}_0$ and $\vec{\mathbf{J}}_p$ respectively. In the former case, equation (23) is therefore an enforcement of the Coulomb gauge, i.e. $\nabla \cdot \vec{\mathbf{A}}_0 = 0$ in Ω in a weak (integrated) sense.

IX. CONCLUSIONS

The method of Albanese and Rubinacci for gauging edge-based vector potential solutions in magnetostatics has been generalized and verified numerically. The resulting formulation, apparently a weak-sense enforcement of the Coulomb gauge, has been shown to apply to direct field solutions of the vector wave equation. It remains to refine and evaluate the method as a possibility for more efficient solution of high frequency problems.

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