An Adjoint Variable Method for Frequency Domain TLM Problems With Conducting Boundaries

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***Abstract*—We propose a novel adjoint variable approach to design sensitivity analysis with the frequency domain transmission line modeling (FDTLM) method. An enlarged system matrix is constructed that includes the perturbed metal sections of the structure. The adjoint system of equations is then formed and solved. The derivatives of the responses with respect to all designable parameters are estimated using two analyses of the original and the adjoint systems. Second-order terms are included by approximating the values of the incident voltage waveforms in the perturbed areas. Our novel technique is illustrated through a number of examples.**

***Index Terms*—Design automation, design methodology, frequency domain analysis, frequency domain transmission line modeling (FDTLM), sensitivity.**

I. Introduction

THE microwave structure design problem can be formulated as

$$\boldsymbol{x}^* = \arg\left\{\min_{\boldsymbol{x}} G(\boldsymbol{x}, \boldsymbol{V}(\boldsymbol{x}))\right\} \tag{1}$$

where $\boldsymbol{x}$ is the vector of designable parameters and $\boldsymbol{V}(\boldsymbol{x})$ is the vector of responses obtained by electromagnetic simulation. G is the objective function to be minimized, and $\boldsymbol{x}^*$ is the vector of optimal designable parameters.

The classical approach for solving (1) treats the electromagnetic simulator as a black box. The derivatives of the responses are obtained through finite differences [1]. For a vector $\boldsymbol{x} \in \Re^n$, one optimization iterate involves $n+1$ full-wave simulations. This significant computational toll motivates research for smarter optimization approaches.

The adjoint variable method (AVM) aims at efficient estimation of the sensitivities of the circuit response with respect to all designable parameters. An adjoint system of equations is constructed and solved. Using the analyses of both the adjoint and original systems, the derivatives of the objective function with respect to all parameters can be estimated [2]–[5].

We suggest a novel implementation of the AVM method in the frequency domain transmission line modeling (FDTLM). The nominal system of equations is first solved for the incident voltage waves. An adjoint system of equations, which is obtained from the original system, is also solved. A small on-grid perturbation in a parameter value is then used to deduce the corresponding perturbation of the system matrix. Efficient estimates of the response sensitivities are obtained using the AVM. The accuracy of these estimates is improved by including an approximate second-order term in the perturbation estimates.

II. FDTLM Method

FDTLM is a method for modeling time-harmonic electromagnetic waves. The computational space is discretized into three-dimensional (3-D) rectangular cells. The FDTLM algorithm [6] utilizes a symmetric condensed cell [7]. Voltage waves incident on each transmission line are scattered to couple to other transmission lines (links). There are 12 incident voltage waves that correspond to the 12 transmission lines. For the jth node, the reflected voltage waves $\boldsymbol{V}^{j,r}$ are related to the vector of incident voltage waves $\boldsymbol{V}^j$ by

$$\boldsymbol{V}^{j,r} = \boldsymbol{S} \cdot \boldsymbol{V}^j \tag{2}$$

where $\boldsymbol{S} \in \Re^{12\times 12}$ is the scattering matrix.

The reflected voltage waves become incident on neighboring cells with the proper delay and transmission factors. The incident voltage waves for all cells are thus obtained by solving the system of linear equations

$$\boldsymbol{A} \cdot \boldsymbol{V} = \boldsymbol{V}^s \tag{3}$$

where $\boldsymbol{A} \in \Re^{12N_t \times 12N_t}$ is the system matrix, $\boldsymbol{V} = [\boldsymbol{V}^{1T} \;\; \boldsymbol{V}^{2T} \cdots \boldsymbol{V}^{N_t T}]^T$ is the vector of incident waves for all cells and the superscript T denotes transpose. $\boldsymbol{V}^s \in \Re^{12N_t}$ is the vector of source excitation with N_t being the total number of cells. The electric and magnetic field phasors are obtained using the solution $\overline{\boldsymbol{V}}$ of (3).

III. AVM Method

The AVM method aims at obtaining response sensitivities with respect to all designable parameters using only two simulations. For a real system of equations $\boldsymbol{A}^R\boldsymbol{V}^R = \boldsymbol{V}^{s,R}$, the adjoint system of equations is given by [4]

$$\boldsymbol{A}^{RT} \cdot \boldsymbol{\lambda}^R = \partial G/\partial \boldsymbol{V}^R. \tag{4}$$

Using the solutions of the original and adjoint systems, the sensitivity of the objective function G with respect to the ith designable parameter is given by [4]

$$\frac{\partial G}{\partial x_i} = \frac{\partial_e G}{\partial x_i} + \boldsymbol{\lambda}^{RT}\left[\frac{\partial \boldsymbol{V}^{s,R}}{\partial x_i} - \frac{\partial \boldsymbol{A}^R}{\partial x_i}\overline{\boldsymbol{V}}^R\right] \tag{5}$$

where $\partial_e/\partial x_i$ is the explicit dependence term. The vector $\overline{\boldsymbol{V}}^R$ is the solution of the original system. Applying this approach to

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the equivalent real system of (3), we obtain the complex adjoint system

$$\boldsymbol{A}^H \cdot \boldsymbol{\lambda} = \left[\frac{\partial G}{\partial \boldsymbol{V}^R} + j\, \frac{\partial G}{\partial \boldsymbol{V}^I} \right] \tag{6}$$

where the superscript H denotes the conjugate transpose, j denotes $\sqrt{-1}$ and $\boldsymbol{V} = \boldsymbol{V}^R + j\boldsymbol{V}^I$.

A major difficulty in applying the AVM approach to the FDTLM is the definition of the term $\partial \boldsymbol{A}/\partial x_i$ for the ith designable parameter, $i = 1, 2, \ldots, n$. A microwave structure is meshed using a rectangular grid of certain dimensions. A designable parameter x_i can assume only a discrete set of values that are multiples of the cell size in its direction. In addition, perturbing the structure would result in a new system matrix with different dimension and thus a meaningful definition of a derivative is not possible. Our novel approach attempts to solve this problem as explained in the following section.

IV. Our Approach

We assume that the structure is discretized for a given set of $\boldsymbol{x}$ values. We limit the discussion to the case where perturbations in parameter values involve only changes in the location of metallic boundaries. For the parameter x_i we assign a corresponding nominal perturbation δx_i. Perturbing the ith parameter by δx_i results in metalizing some cells and demetalizing other cells. We denote the set of indices of metalized and demetalized cells by $S_{m,\,i}$ and $S_{d,\,i}$, respectively. The system matrix $\boldsymbol{A}$ is constructed and the system of (3) is solved to obtain the vector $\overline{\boldsymbol{V}}$. For the ith parameter we define the corresponding enlarged system of equations

$$\boldsymbol{A}_i \boldsymbol{V}_i = \boldsymbol{V}_i^s \tag{7}$$

where

$$\boldsymbol{A}_i = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \end{bmatrix},\ \boldsymbol{V}_i = \begin{bmatrix} \boldsymbol{V} \\ \boldsymbol{V}_{d,\,i} \end{bmatrix},\ \boldsymbol{V}_i^s = \begin{bmatrix} \boldsymbol{V}^s \\ \boldsymbol{0} \end{bmatrix} \tag{8}$$

where $\boldsymbol{I} \in \Re^{12N_{d,\,i} \times 12N_{d,\,i}}$ is the identity matrix and $N_{d,\,i}$ is the cardinality of $S_{d,\,i}$. Here, we include the vector $\boldsymbol{V}_{d,\,i}$ of incident voltage waves related to the cells in the set $S_{d,\,i}$. The solution to (7) is $\overline{\boldsymbol{V}}_i = [\overline{\boldsymbol{V}}^T\ \ \boldsymbol{0}^T]^T$. Metalizing the cells in the set $S_{m,\,i}$ and demetalizing the cells in $S_{d,\,i}$ result in an overall perturbation $\Delta \boldsymbol{A}_i$ of the enlarged system matrix.

The perturbed system of equations is thus given by

$$(\boldsymbol{A}_i + \Delta \boldsymbol{A}_i)\left(\overline{\boldsymbol{V}}_i + \Delta \boldsymbol{V}_i\right) = \boldsymbol{V}_i^s \tag{9}$$

where $\Delta \boldsymbol{V}_i$ is the unknown change in the vector of incident voltage waves due to the perturbation δx_i. Here, we assume that the sources are unaffected by any perturbation δx_i. Simplifying (9) we get

$$\boldsymbol{A}_i \Delta \boldsymbol{V}_i = -\Delta \boldsymbol{A}_i \overline{\boldsymbol{V}}_i - \Delta \boldsymbol{A}_i \Delta \boldsymbol{V}_i. \tag{10}$$

A number of important notes should be made with regard to (10). First, the matrix $\Delta \boldsymbol{A}_i$ contains very few nonzero components corresponding to the links in the sets $S_{m,\,i}$, $S_{d,\,i}$ and the neighboring connecting links. Second, to simplify the approach, the second-order term $\Delta \boldsymbol{A}_i \Delta \boldsymbol{V}_i$ could be neglected. This, however, reduces the accuracy of our sensitivity estimates because the nonzero components of $\Delta \boldsymbol{A}_i$ are of the same order of magnitude as the corresponding components of $\boldsymbol{A}_i$. This prompts us to approximate the components of the vector $\Delta \boldsymbol{V}_i$ corresponding to the nonzero columns of $\Delta \boldsymbol{A}_i$ in the right hand side of (10). Some of these components are already known. The perturbations in the incident voltage waves distribution of the links in $S_{m,\,i}$ are given by

$$\Delta \boldsymbol{V}_{i,\,k} = -\overline{\boldsymbol{V}}_k, \qquad \forall\, k \in S_L(M),\ M \in S_{m,\,i} \tag{11}$$

where $S_L(M)$ is the set of link indices associated with the Mth cell. For all other cells, we exploit perturbation theory and assume that the field distribution in the neighborhood of the perturbed cells is very close to the field distribution at corresponding cells of the unperturbed structure. We approximate the values of the incident voltage waves using a one-to-one mapping between the perturbed and unperturbed structure. This approach is illustrated in Fig. 1.

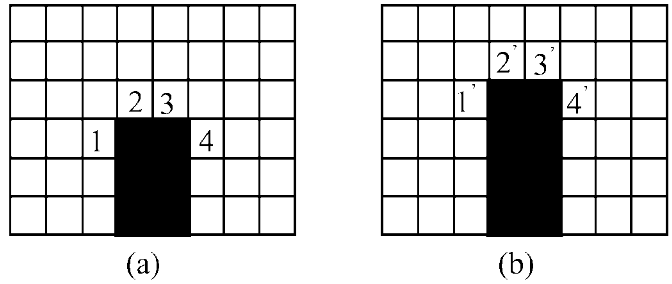

Fig. 1. Approximation of the values of the incident voltage waves in the neighborhood of the perturbed structure: the incident wave values in the cells 1′, 2′, 3′ and 4′ of the perturbed structure are approximated by the corresponding values in the cells 1, 2, 3, and 4 of the unperturbed structure.

It follows that we can define

$$\boldsymbol{\eta}_i = -\Delta \boldsymbol{A}_i \overline{\boldsymbol{V}}_i - \Delta \boldsymbol{A}_i \Delta \widehat{\boldsymbol{V}}_i = \begin{bmatrix} \boldsymbol{Q}_i \\ \boldsymbol{W}_i \end{bmatrix} \tag{12}$$

where $\Delta \widehat{\boldsymbol{V}}_i$ contains the approximate values with zeros in all other components and $\boldsymbol{W}_i \in \Re^{12 \times N_{d,\,i}}$. Following similar derivation for that given in [4], [5] we see that

$$\Delta G = \frac{\partial_e G}{\partial x_i}\,\delta x_i + \begin{bmatrix} \boldsymbol{\lambda}_i^R \\ \boldsymbol{\lambda}_i^I \end{bmatrix}^T \begin{bmatrix} \boldsymbol{\eta}_i^R \\ \boldsymbol{\eta}_i^I \end{bmatrix} \tag{13}$$

where $\boldsymbol{\lambda}_i = [\boldsymbol{\lambda}^T\ \ \boldsymbol{0}^T]^T$ and $\boldsymbol{\lambda}$ is obtained by solving (6). The first-order derivative of the objective function with respect to the ith parameter is thus approximated by

$$\frac{\partial G}{\partial x_i} \approx \frac{\Delta G}{\delta x_i} = \frac{\partial_e G}{\partial x_i} + \frac{1}{\delta x_i} \begin{bmatrix} \boldsymbol{\lambda}^R \\ \boldsymbol{\lambda}^I \end{bmatrix}^T \begin{bmatrix} \boldsymbol{Q}_i^R \\ \boldsymbol{Q}_i^I \end{bmatrix}. \tag{14}$$

V. Examples

A. Sensitivities of a Septum

We consider estimating the sensitivity of $|S_{21}|^2$ with respect to the septum length L (see Fig. 2). This problem is solved as a two-dimensional (2-D) problem by invoking electrical walls at the top and bottom planes of the computational domain. A square cell of dimension $\Delta x = 0.0025$ m is utilized. The waveguide length and width are $30\Delta z$ and $20\Delta x$, respectively. The length at which sensitivities are evaluated is $L_0 = 4\Delta x$.

We compare the sensitivities estimated using our approach with those obtained using central differences applied directly to

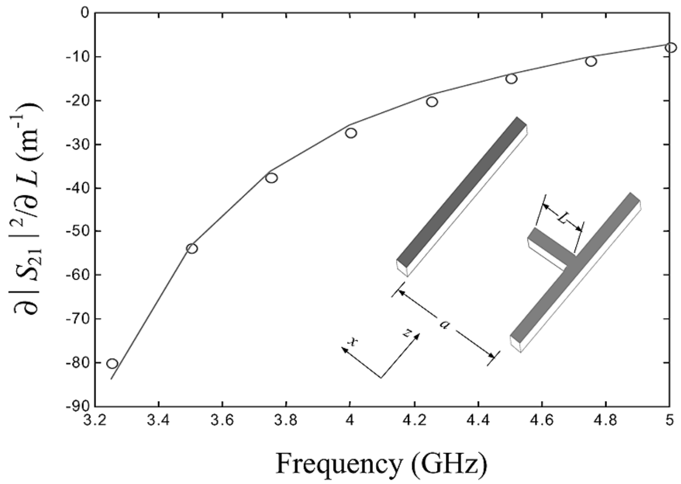

Fig. 2. Comparison between the sensitivity $\partial |S_{21}|^2/\partial L$ obtained using central differences (o) and using our discrete AVM approach (—) for the septum example.

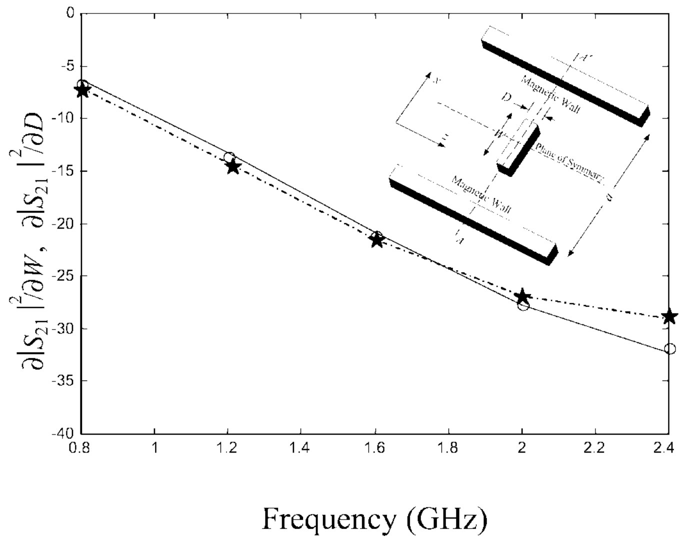

Fig. 3. Comparison between the different sensitivities for the inductive obstacle example; $\partial |S_{21}|^2/\partial W$ obtained using central differences (o) and using our discrete AVM approach (—) and $\partial |S_{21}|^2/\partial D$ obtained using central differences ($*$) and using our discrete AVM approach (- - -).

the response function $|S_{21}|^2$ over a range of frequencies (see Fig. 2). A good agreement is obtained.

B. Sensitivities of an Inductive Obstacle in a Waveguide

We also consider the sensitivities of $G = |S_{21}|^2$ of an inductive obstacle in a parallel plate waveguide shown in Fig. 3. A square cell of dimensions $\Delta x = 0.002$ m is used. We solve this problem as a 2-D problem for the dominant mode. The waveguide length and width are $31\Delta z$ and $30\Delta x$, respectively. Symmetry is exploited to simulate only half of the waveguide volume. The vector of parameters is $\boldsymbol{x} = [W \quad D]^T$.

We estimate the sensitivities of the response with respect to the parameters at a number of frequencies. These sensitivities are estimated at $\boldsymbol{x} = [6\Delta x \quad 3\Delta z]^T$. A symmetric set $S_{m,2}$ is used for the parameter D. Our results are compared with those obtained using central differences. The results are shown in Fig. 3. Very good agreement is obtained.

VI. CONCLUSIONS

We present a novel discrete adjoint variable method for sensitivity analysis with the FDTLM. An enlarged system matrix enables us to define a perturbation matrix for each parameter. The accuracy of our sensitivity estimates are improved by including an approximate second-order term in the analysis. The method is easy to implement as it requires neither changes in the meshing procedure nor changes in the grid size. Our approach was tested through two examples involving metallic obstacles. Very good match is obtained between our sensitivities and those obtained using the computationally expensive central differences.

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