An Adjoint Variable Method for Time Domain TLM with Fixed Structured Grids

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Abstract — **We present a breakthrough algorithm for efficient estimation of objective function sensitivities for time-domain TLM with nondispersive boundaries. The original electromagnetic structure is simulated using TLM. An adjoint TLM simulation that runs backward in time is derived and solved. The sensitivities of the objective function with respect to all the designable parameters are estimated using only the original and adjoint simulations. Our approach is illustrated through estimating the sensitivities of an objective function with respect to the dimensions of a waveguide discontinuity.**

I. INTRODUCTION

The traditional design problem of a microwave structure can be formulated as

$$x^* = arg\left\{\min_{x} \; F(x, R(x))\right\} \tag{1}$$

where x is the vector of designable parameters and $R(x)$ is the vector of responses obtained by electromagnetic simulation. F is the objective function to be minimized and x^* is the vector of optimal designable parameters.

Classical optimization approaches for solving (1) with a finely discretized electromagnetic simulator ("fine" model) can be prohibitive. This motivates research for more efficient optimization approaches. Space Mapping [1], for example, exploits the existence of another fast but less accurate "coarse" model of the circuit under consideration. In [2] an analytical expression is derived for the admittance matrix of a finite element analysis of a microstrip circuit. Another approach [3] derives the current derivatives integral equation. The derivatives are then expanded in terms of the same basis functions used in the analysis. The same LU decomposed analysis matrix is reused to solve for the derivatives coefficients.

Another alternative is to utilize adjoint variable methods [4]. Using only two analyses of the original and adjoint circuits, the sensitivities with respect to all the designable parameters can be obtained. This method was mainly developed for network and control theories. Recent research attempts to apply this approach to the Method of Moments (MoM) [5], Frequency Domain Transmission Line Modeling (FDTLM) [6] and the FDTD method with unstructured grids [7].

Several approaches are suggested for efficient optimization using time-domain TLM. For example, the algorithm suggested in [8] exploits the time reversal property of the TLM method [9]. The impulses corresponding to a desired response are obtained through inverse Fourier transform. These impulses are then propagated back in time to determine the geometry of the designable discontinuity. This inversion process, however, may not produce a unique result. A more recent approach [10] is developed for the synthesis of a microwave structure. The designable parameters are associated with a set of characteristic frequencies. The design specifications determine the desired values of these frequencies. A synthesis phase is then carried out for each parameter. In this phase, the corresponding optimizable boundary parts are replaced by matched sinusoidal sources. The new geometry is determined by observing the envelope of the electric/magnetic field inside the structure.

In this paper, we present a novel Adjoint Variable Method (AVM) approach to design sensitivity analysis with time-domain TLM. An adjoint structure is derived from the original structure. Both the original and adjoint structures are simulated. The incident and adjoint impulses are stored during these simulations only at few mesh links related to each designable parameter. Using only two simulations, of the original and the adjoint structures, the sensitivities of the objective function with respect to all designable parameters can be obtained.

II. THE TLM METHOD

The TLM method carries out a sequence of scattering and connection steps [9]. For the jth non-metalized node the scattering relation is given by

$$V_k^{R,j} = S^j V_k^j \tag{2}$$

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where V_k^j is the vector of incident impulses on the jth node at the kth time step, $V_k^{R,j}$ is the vector of reflected impulses of the jth node at the same time step, and S^j is the scattering matrix of the jth node. The reflected impulses from each node become incident on neighboring nodes at the next time step. It follows that one TLM step is given by

$$V_{k+1} = C\,S V_k + V_k^s \tag{3}$$

where V_k is the vector of incident impulses for all nodes $V_k = \left[V_k^{1T} \;\; V_k^{2T} \;\; \cdots \;\; V_k^{NT}\right]^T$ and the superscript T denotes the transpose. Here, we assume that the computational domain is discretized into a total of N non-metalized nodes with node size Δl. The matrix S is a block diagonal matrix whose jth diagonal block is S^j. C is the connection matrix describing how reflected impulses connect to neighboring nodes/boundaries. The vector V_k^s is the vector of source excitation at the kth time step.

III. Our AVM Approach

The goal is to efficiently estimate the gradient of the objective function with respect to the designable parameters x at a given set of values x^0. The objective function that we consider is of the form [7]

$$F = \int_0^{T_m}\int_\Omega G(x,V)\, d\Omega\, dt \tag{4}$$

where Ω is the observation domain, V is the corresponding continuous vector of V_k, and T_m is the maximum simulation time. The analytic derivative of this objective function with respect to the ith parameter is given by

$$\frac{\partial F}{\partial x_i} = \int_0^{T_m}\int_\Omega \frac{\partial^e G}{\partial x_i} d\Omega\, dt + \int_0^{T_m}\int_\Omega \left(\frac{\partial G}{\partial V}\right)^T \frac{\partial V}{\partial x_i} d\Omega\, dt \tag{5}$$

where $\frac{\partial^e}{\partial x_i}$ denotes the explicit dependence.

For a band-limited excitation and for sufficiently small time step Δt, equation (3) can be expressed as

$$V_k + \left(\frac{\partial V}{\partial t}\right)_k \Delta t \approx C S V_k + V_k^s \tag{6}$$

Simplifying (6) we get

$$\frac{\partial V}{\partial t} = A(x)V + \frac{V^s}{\Delta t} \tag{7}$$

where $A(x) = \frac{1}{\Delta t}\left(C(x)S(x) - I\right)$ and I is the identity matrix. Notice that in (7) we omitted the subscript k to denote an arbitrary time not only multiples of Δt.

We limit ourselves to the case where perturbing one of the parameters x_i by Δx_i results in metalizing some of the nodes. Here, Δx_i is selected as the smallest on-grid perturbation of the ith parameter. This causes a perturbation ΔA_i of the matrix A. From (7) we obtain

$$\frac{\partial^2 V}{\partial t \partial x_i} \approx \frac{\partial A}{\partial x_i} V + A\frac{\partial V}{\partial x_i} + \Delta A_i \frac{\partial V}{\partial x_i} \tag{8}$$

The second order term in (8) should not be neglected. This is because the perturbation in the connection and scattering matrices is of the same order of magnitude as their values. Notice also in (8) that the excitation is assumed independent of the designable parameters.

Following a similar approach to [7], we define the adjoint variable λ through the equation

$$\int_0^{T_m} \lambda^T \left(\frac{\partial^2 V}{\partial t \partial x_i} - \frac{\partial A}{\partial x_i} V - A\frac{\partial V}{\partial x_i} - \Delta A_i \frac{\partial V}{\partial x_i}\right) dt = 0 \tag{9}$$

Integrating (9) by parts we get

$$\lambda^T \frac{\partial V}{\partial x_i}\Bigg|_0^{T_m} - \int_0^{T_m} \left(\frac{d\lambda^T}{dt} + \lambda^T (A + \Delta A_i)\right)\frac{\partial V}{\partial x_i} dt = \int_0^{T_m} \lambda^T \frac{\partial A}{\partial x_i} V\, dt \tag{10}$$

The adjoint variable λ is selected to have a terminal value of $\lambda(T_m) = \mathbf{0}$. Also, the vector V has an initial zero value regardless of the value of the parameter x_i, i=1, 2, …, n. It follows that the first term in (10) vanishes. Equation (10) can thus be written as

$$\int_0^{T_m} \left(\frac{d\lambda^T}{dt} + \lambda^T (A + \Delta A_i)\right)\frac{\partial V}{\partial x_i} dt = -\int_0^{T_m} \lambda^T \frac{\partial A}{\partial x_i} V\, dt \tag{11}$$

Comparing the second term in (5) with the left hand side of (11), we choose

$$\frac{d\lambda^T}{dt} + \lambda^T (A + \Delta A_i) = \left(\frac{\partial G}{\partial V}\right)^T \tag{12}$$

Using the definition of the matrix A, we write (12) in discrete time as

$$\lambda_{k-1} = S^\lambda C^\lambda \lambda_k - V_k^{s,\lambda}, \;\; \lambda(T_m) = \mathbf{0} \tag{13}$$

where $S^\lambda = S^T(x + \Delta x_i e_i)$ is the scattering matrix of the adjoint system, $C^\lambda = C^T(x + \Delta x_i e_i)$ is the connection matrix of the adjoint system and $V_k^{s,\lambda} = \left(\frac{\partial G}{\partial V}\right)_{t=k\Delta t}$ is the adjoint excitation.

Equation (13) represents a TLM simulation that is running backward in time with known excitation. This simulation provides the value of the adjoint variable λ at all time steps. Using (5), (11) and (12), the sensitivity of F with respect to the ith parameter is given by

$$\frac{\partial F}{\partial x_i} = \frac{\partial^e F}{\partial x_i} - \int_0^{T_m} \lambda^T \frac{\partial \boldsymbol{A}}{\partial x_i} \boldsymbol{V}\, dt \approx \frac{\partial^e F}{\partial x_i} - \Delta t \sum_k \lambda_k^T \frac{\Delta \boldsymbol{A}_i}{\Delta x_i} \boldsymbol{V}_k \qquad (14)$$

The matrix $\Delta \boldsymbol{A}_i$ in (14) contains only few nonzero elements. So we need only store the impulses for the original and adjoint problems for small number of mesh links at all time steps.

The main difficulty in applying (14) is that the adjoint problem in (13) is solved for the perturbed problem, which is parameter-dependent. To overcome this, we assume that the perturbation done in each parameter is small and does not affect in a significant way the distribution of the incident impulses. The adjoint impulses required in (14) are approximated by the values of the corresponding incident impulses for the unperturbed adjoint problem:

$$\lambda_{k-1} = \boldsymbol{S}^T(\boldsymbol{x})\boldsymbol{C}^T(\boldsymbol{x})\lambda_k - \boldsymbol{V}_k^{s,\lambda},\ \lambda(T_m) = \boldsymbol{0} \qquad (15)$$

Our experience shows that this approximation introduces very little error if Δx_i is sufficiently small. This approximation is illustrated for 2D TLM in Fig. 1.

Our AVM algorithm can thus be summarized in the following steps.

1. *Parameterization*: determine the sets of link indices L_i whose connection and scattering matrices are affected by the perturbations Δx_i, i=1, 2,…, n.
2. *Original Analysis*: carry out the original TLM analysis (3) and store the set of impulses for all indices in the set L_i, i=1, 2,…, n. The values of the incident impulses in the observation domain are also stored to determine the adjoint excitation.
3. *Adjoint Analysis*: carry out the backward adjoint analysis (15) with the adjoint excitation determined in step 2. Store the impulses of the links with indices L_i, i=1, 2,…, n.
4. *Sensitivities Estimation*: evaluate (14) for all parameters.

IV. EXAMPLES

We illustrate our AVM technique through estimating the sensitivities for an inductive obstacle in the parallel plate waveguide shown in Fig. 2. The width of the waveguide is a = 6.0 cm. The length of the waveguide is d = 6.2 cm. A square cell of dimension Δl = 0.002 m is utilized. This problem is simulated as a 2D problem with a Gaussian-modulated sinusoidal excitation of frequency f = 2.0 GHz. Symmetry is employed to simulate only half of the structure. The objective function is taken as

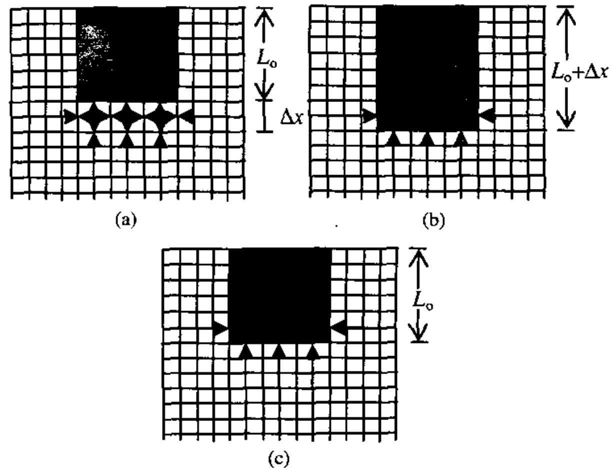

Fig. 1. Illustration of the links storage; a) the arrowed links are the ones for which the matrix ΔA has nonzero components for a perturbation of $1\Delta x$ of the parameter L, b) the arrowed links are the ones that should be stored during the adjoint analysis of the perturbed circuit and c) the links in (b) are approximated by their corresponding ones for the unperturbed circuit.

$$F(\boldsymbol{x},\boldsymbol{V}) = \frac{\int_0^{T_m}\int_\Omega e_y^2\, dx dt}{\Delta l} \qquad (16)$$

where Ω is the cross section of the waveguide at the last column of nodes and e_y is the y component of the electric field which is a function of the incident impulses. The objective function (16) is approximated by

$$F(\boldsymbol{x},\boldsymbol{V}) = \Delta t \sum_{k=1}^{N_t} \sum_{i=1}^{N_x} e_{yk}^2(i, N_z) \qquad (17)$$

where N_x is the number of cells in the x direction and N_t is the number of time steps.

The gradient of this objective function is estimated using our AVM approach for different sets of parameters' values. The comparison between the AVM results and the central difference derivatives is shown in Fig. 3. We see that the error introduced by utilizing the approximation (15) is acceptable for optimization purposes. Incorporating a finer grid (Δl = 1.0 mm) results in a reduced error in the AVM gradients as shown in Fig. 4 because the approximation (15) becomes more valid for a finer grid.

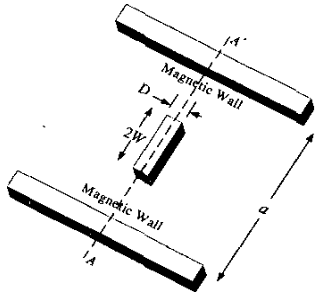

Fig. 2. The inductive obstacle example.

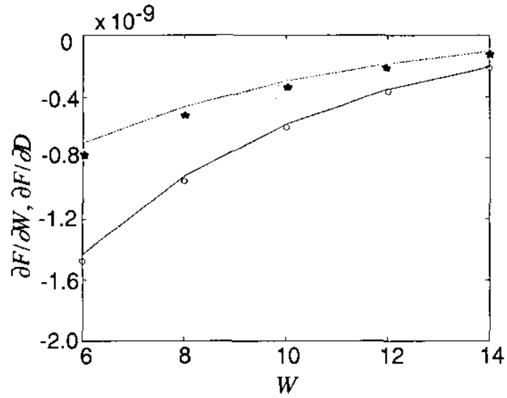

Fig. 3. Objective sensitivities for the inductive obstacle example at $D = 3\Delta l$ with $\Delta l = 2.0$ mm for different values of W; $\partial F/\partial W$ obtained using AVM (—), $\partial F/\partial W$ obtained using central differences (o), $\partial F/\partial D$ obtained using AVM (--) and $\partial F/\partial D$ obtained using central differences (*).

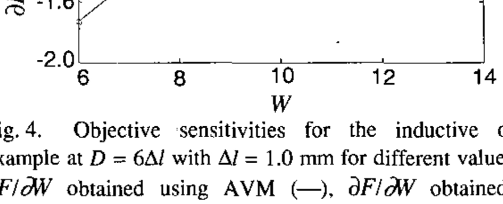

Fig. 4. Objective sensitivities for the inductive obstacle example at $D = 6\Delta l$ with $\Delta l = 1.0$ mm for different values of W; $\partial F/\partial W$ obtained using AVM (—), $\partial F/\partial W$ obtained using central differences (o), $\partial F/\partial D$ obtained using AVM (--) and $\partial F/\partial D$ obtained using central differences (*).

V. Conclusions

For the first time, an adjoint variable approach is presented for efficient sensitivities estimation in the TLM method. An adjoint TLM simulation that runs backward in time is set up using the original structure. Using only these two simulations, the derivatives of the objective function with respect to all designable parameters are estimated. The proposed technique features simplicity and excellent accuracy. Its implementation with existing TLM algorithms is straight-forward. Our approach is illustrated through a waveguide discontinuity example.

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