EXTRACTING THE DERIVATIVES OF NETWORK PARAMETERS FROM FREQUENCY-DOMAIN ELECTROMAGNETIC SOLUTIONS

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Abstract: We present a methodology for extracting the gradients of the network parameters in the design parameter space from full-wave high-frequency solutions provided by commercial electromagnetic (EM) solvers. We consider frequency-domain solvers. We show that the derivatives of network parameters such as the *Y*-, *Z*-, and *S*-parameters can be obtained from the full-wave solution with little overhead. Our approach exploits the theory of adjoint sensitivity analysis applied to self-adjoint problems. When the system matrix generated by the solver is symmetric (self-adjoint), such as in the finite-element method, the approach is unconditionally applicable. For the method of moments, which usually generates an asymmetric system matrix, it is applicable with a convergent solution. Our method requires that the solver gives access to: 1) the system matrix, and 2) the solution vector. Also, the user needs to have limited control over the meshing such that the mesh size and structure do not change as shape design parameters are perturbed. The design parameters may relate to both the shape and the materials of the structure. The gradient information is intended for gradient-based optimization, advanced modeling techniques, and for tolerance analysis.

I. ADJOINT SENSITIVITY ANALYSIS: BACKGROUND

In traditional electromagnetic (EM) analysis, the behaviour of a system or structure is described by a set of responses, e.g., its *S*-parameters. The design sensitivity consists of the response derivatives with respect to shape or material parameters. When added to the responses, this derivative information is of great value for the purposes of optimization, modelling, yield and tolerance analyses, or the design of experiments.

The sensitivity of a response function f with respect to a set of N design parameters $\boldsymbol{p}=[p_1\ \ p_2\ \ \cdots\ \ p_N]^T$ is given by its gradient,

$$\nabla_{\boldsymbol{p}} f = \left[\frac{\partial f}{\partial p_1}\ \ \frac{\partial f}{\partial p_2}\ \ \cdots\ \ \frac{\partial f}{\partial p_N} \right]. \tag{1}$$

The response f may be a real-valued scalar as in the case of an optimization problem, or it may be a complex scalar, e.g., a network parameter, as in the case of modeling. In the latter case, we often deal with a set of responses. The response is calculated from the full-wave solution, which is obtained by solving the linear problem (in the case of linear materials)

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}\ . \tag{2}$$

Here, $\boldsymbol{A}$ is the system matrix, $\boldsymbol{x}$ is the vector of state variables (field or current density solution), and $\boldsymbol{b}$ is the excitation vector resulting from volume sources or inhomogeneous boundary conditions. The linear system describing the high-frequency EM problem is complex. Thus, the response f is a function of the field solution $\boldsymbol{x}$, and, through it, it is an implicit function of the design parameters $\boldsymbol{p}$. It may also be an explicit function of $\boldsymbol{p}$.

The sensitivity of a complex-valued response $f\left(\boldsymbol{x}(\boldsymbol{p}), \boldsymbol{p}\right)$, $f = f_R + jf_I$ ($j=\sqrt{-1}$), is given by [1][2]

$$\nabla_{\boldsymbol{p}} f = \nabla^e_{\boldsymbol{p}} f + \hat{\boldsymbol{x}}^T \cdot \left[\nabla_{\boldsymbol{p}} \boldsymbol{b} - \nabla_{\boldsymbol{p}} (\boldsymbol{A}\bar{\boldsymbol{x}}) \right] \tag{3}$$

provided that it is an analytic function of the state variables in $\boldsymbol{x}$. The gradient $\nabla^e_{\boldsymbol{p}} f$ contains the derivatives due to the explicit dependence of f on the design parameters. Here, $\bar{\boldsymbol{x}}$ is the solution of $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ at the current design, while $\hat{\boldsymbol{x}}$ is the solution to

$$\boldsymbol{A}^T \hat{\boldsymbol{x}} = \hat{\boldsymbol{b}} \tag{4}$$

(the adjoint problem) at the current design. In (4), $\hat{\boldsymbol{b}}=[\nabla_{\boldsymbol{x}} f(\bar{\boldsymbol{x}})]^T = [\nabla_{\mathrm{Re}\boldsymbol{x}} f_R(\bar{\boldsymbol{x}}) + j\nabla_{\mathrm{Re}\boldsymbol{x}} f_I(\bar{\boldsymbol{x}})]^T$. Note that $\hat{\boldsymbol{b}}$ is calculated at the solution $\bar{\boldsymbol{x}}$. If f is real-valued, then [1][3]

$$\nabla_{\boldsymbol{p}} f = \nabla^e_{\boldsymbol{p}} f + \mathrm{Re}\left\{ \hat{\boldsymbol{x}}^T \cdot \left[\nabla_{\boldsymbol{p}} \boldsymbol{b} - \nabla_{\boldsymbol{p}} (\boldsymbol{A}\bar{\boldsymbol{x}}) \right] \right\} \tag{5}$$

with $\hat{\boldsymbol{b}} = [\nabla_{\mathrm{Re}\boldsymbol{x}} f - j\nabla_{\mathrm{Im}\boldsymbol{x}} f]^T$. If f is complex valued but not analytic, its real and imaginary parts f_R and f_I are treated as separate responses requiring the solution of two respective adjoint problems in the form of (5). The term $\nabla_{\boldsymbol{p}}(\boldsymbol{A}\bar{\boldsymbol{x}})$ is written in an expanded form as $(\partial \boldsymbol{A}/\partial p_n)\cdot \bar{\boldsymbol{x}}$, $n=1,\ldots,N$, where the matrices $\partial \boldsymbol{A}/\partial p_n$ can be found either by finite differences or by an iterative Broyden approximation in the case of optimization applications [3]. The calculation of this term requires that the EM solver can export: 1) the $\boldsymbol{A}$ matrix, and 2) the solution vector $\bar{\boldsymbol{x}}$.

II. SENSITIVITY ANALYSIS OF SELF-ADJOINT PROBLEMS

A self-adjoint problem is characterized by a symmetric system matrix, $\boldsymbol{A}=\boldsymbol{A}^T$. In the case of complex analysis, formally, the system is self-adjoint if $\boldsymbol{A}=\boldsymbol{A}^H=\boldsymbol{A}^{*T}$. For the purposes of sensitivity analysis, however, the condition $\boldsymbol{A}=\boldsymbol{A}^T$ is also acceptable. From (2) and (4), it is obvious that the original and adjoint systems of equations share the same (or conjugated) system matrix if the problem is self-adjoint. The implications of the self-adjoint property of a system in its sensitivity analysis become important when the response f is such that the adjoint excitation vector $\hat{\boldsymbol{b}}=[\nabla_{\boldsymbol{x}} f(\bar{x})]^T$ relates to the original excitation vector $\boldsymbol{b}$ as

$$\hat{\boldsymbol{b}}=\kappa\boldsymbol{b} \tag{6}$$

where κ is a complex constant. Due to the linear nature of the problem in (4), we conclude that the adjoint solution vector $\hat{\boldsymbol{x}}$ is obtained from the original solution $\boldsymbol{x}$ as

$$\hat{\boldsymbol{x}}=\kappa\boldsymbol{x} \tag{7}$$

and there is no need to solve separately the adjoint quasi-EM problem in (4). This is important since the solution of the adjoint problem may be computationally equivalent to one full-wave analysis, e.g., when the linear systems (2) and (4) are solved with iterative methods. When (7) holds, the sensitivity formula becomes

$$\nabla_{\boldsymbol{p}} f = \nabla^e_{\boldsymbol{p}} f + \kappa\bar{\boldsymbol{x}}^T \cdot \left[\nabla_{\boldsymbol{p}}\boldsymbol{b} - \nabla_{\boldsymbol{p}}(\boldsymbol{A}\bar{\boldsymbol{x}})\right]. \tag{8}$$

The same simplification applies to (5). We later show that in the case of network parameters, the adjoint excitation vectors fulfill (6).

When the response f is a network parameter, it does not have an explicit dependence on the design parameters. Explicit dependence on a shape parameter p_i ($\partial^e f/\partial p_i \neq 0$) arises when f depends on the field/current solution at points whose coordinates in space are affected by a change in p_i. An example is the explicit dependence of an antenna gain on the position/shape of the wires carrying the radiating currents [4]. Explicit dependence with respect to a material parameter arises when f depends on the field/current solution at points whose constitutive parameters are affected by its change. An example is the stored energy in a volume of changing permittivity. The network parameters, however, are computed from the solution at the ports, whose shape and materials do not change. Thus, when f is a network parameter, $\nabla^e_{\boldsymbol{p}} f = \mathbf{0}$. In addition, in a problem of finding the sensitivities of network parameters, the excitation vector $\boldsymbol{b}$ is independent of $\boldsymbol{p}$, because the waveguide structures (the ports) launching the incident waves serve as a reference and are not a subject to design changes: $\nabla_{\boldsymbol{p}}\boldsymbol{b}=\mathbf{0}$. Thus, for a network parameter, the sensitivity formula is

$$\nabla_{\boldsymbol{p}} f = -\kappa\bar{\boldsymbol{x}}^T \cdot \nabla_{\boldsymbol{p}}(\boldsymbol{A}\bar{\boldsymbol{x}}). \tag{9}$$

Next, we derive the constant κ in the case of S-parameter and input-impedance sensitivity calculations.

1. *S*-parameters in Finite-element Solutions

The finite-element EM solvers compute the electric field in the whole computational volume. The S-parameters are calculated from the field at the planes of the ports. The S_{kj} parameter can be expressed as

$$S_{kj}^{(\upsilon)} = \frac{\iint\limits_{k\text{-port}} (\mathbf{a}_n \times \mathbf{E}_j^{(\upsilon)})\cdot(\mathbf{a}_n \times \mathbf{e}_k^{(\upsilon)})ds_k}{\iint\limits_{j\text{-port}} (\mathbf{a}_n \times \mathbf{E}_j^{(\upsilon)inc})\cdot(\mathbf{a}_n \times \mathbf{e}_j^{(\upsilon)})ds_j}\cdot\sqrt{\frac{Z_j}{Z_k}} - \delta_{kj}\,,\ \delta_{kj}=\begin{cases}1, & k=j\\ 0, & k\neq j\end{cases} \tag{10}$$

where the jth port is excited and all other ports are matched. The kth port is where the transmitted/reflected field is recorded. The superscript (υ) denotes the mode of interest. $\mathbf{E}_j^{(\upsilon)}$ is the field resulting from the jth port being excited with the υ mode. $\mathbf{E}_j^{(\upsilon)inc}=E_0\mathbf{e}_j^{(\upsilon)}$ is the incident field at the jth port exciting the υ mode. E_0 is usually set equal to 1. At each port, we are interested in the transverse field components. This is why we take the cross product with the unit normal $\mathbf{a}_n$ to the port surface. The modal vector $\mathbf{e}_\xi^{(\upsilon)}$ ($\xi=j,k$) of each port [5] is a real vector when propagating modes are considered. The modal vectors of each port form an orthonormal set. They are obtained either analytically or numerically [5][6][7]. The analytical expressions for the modes $\mathbf{e}^{(\upsilon)}$ of some popular waveguides can be found in [5]. Finally, to obtain the generalized S-parameter, the waveguide impedances Z_j and Z_k of the respective ports must be taken into account.

Note that in order to obtain the whole scattering matrix of a K-port structure, K full-wave analyses are carried out – each port is excited with the desired mode while all other ports are matched. This corresponds to K solutions of (2) with K different right-hand sides, $\boldsymbol{b}_k$, $k=1,\ldots,K$, which results in K field solutions, $\boldsymbol{x}_k \leftrightarrow \mathbf{E}_k(x,y,z)$.

Using the above definition, we differentiate S_{kj} with respect to the field at the kth port, and obtain the respective adjoint excitation vector $\hat{\boldsymbol{b}}_{kj}$ as

$$\hat{\boldsymbol{b}}_{kj} = \frac{\sqrt{Z_j / Z_k}}{2\gamma_k E_0 \iint\limits_{j\text{-port}} (\mathbf{a}_n \times \mathbf{E}_j^{inc}) \cdot (\mathbf{a}_n \times \mathbf{e}_j) ds_j} \cdot \boldsymbol{b}_k \, . \quad (11)$$

Here, $\boldsymbol{b}_k$ is the excitation vector of the original problem when the *k*th port is excited, and γ_k is the propagation constant of the *k*th port. The superscript (υ) has been omitted to simplify notations. This defines the set of complex constants κ_{kj} in the case of the *S*-parameter sensitivities with finite-element solutions for use with the self-adjoint formula (9).

2. *S*-parameters with the Method of Moments (MoM)

Similarly to the case of the FEM solution considered above, with the MoM, the *S*-parameters depend on the current density solutions through simple linear relations. More specifically, the current solution at the ports is needed. Consider the calculation of the *S*-parameters of a network of system impedance Z_0:

$$S_{kj} = \delta_{kj} - \frac{2Z_0 I_{k,j}}{V_j^e}, \;\; j,k = 1,\ldots,K \, . \quad (12)$$

Here, V_j^e is the *j*th port voltage source of internal impedance Z_0 (usually $V_j^e = 1$), and $I_{k,j}$ is the resulting current at the *k*th port when the *j*th port is excited (the rest of the ports are loaded with Z_0). The right-hand side of (2) corresponding to V_j^e exciting the *j*th port is $\boldsymbol{b}_j$. In the case of wire antennas, the port currents $I_{k,j}$ are elements of the solution vector $\boldsymbol{x}_j$. In the case of surface current density solutions, the port currents are linear functions of the current densities at the *k*th port. Taking the derivative of S_{kj} with respect to these current densities, we obtain the adjoint excitation vectors as

$$\hat{\boldsymbol{b}}_{kj} = -\frac{2Z_0}{V_k^e V_j^e} \boldsymbol{b}_k \, , \;\; j,k = 1,\ldots,K \, . \quad (13)$$

Equation (13) defines the constants of the self-adjoint sensitivity expression as $\kappa_{kj} = -2Z_0 / (V_k^e V_j^e)$ for use with (9).

In the case of the input impedance Z_{in}, the constant is found as $\kappa = -I_{in}^2$ where I_{in} is the *complex* current at the port.

III. RESULTS AND DISCUSSION

We apply the self-adjoint sensitivity analysis to a number of examples and compare them with the sensitivity result obtained by forward finite-difference approximation. The results of the two methods are denoted as FFD (forward finite-difference) and SASA (self-adjoint sensitivity analysis), respectively. We emphasize that the FFD approximation of the response gradient requires *N* additional simulations, where *N* is the number of design parameters. Our technique is significantly more efficient in terms of CPU time.

1. Results with the Finite-Element Method (FEMLAB [8])

Here, we present an example of a direct coupled dielectric resonator filter. It is analyzed for the dominant TE_{10} mode. The structure of the filter is shown in Fig. 1. It consists of two resonator blocks of a high relative dielectric constant $\varepsilon_r = 9.6$, which are separated by a coupling section of air with $\varepsilon_r = 1$. The design parameters are the length of the resonator blocks normalized to the waveguide width s/a, and the length of the coupling section normalized to the waveguide width d/a. We compute the S_{21} derivatives at a frequency of 2.1 GHz. We fix s/a at 0.48 while the range of d/a is from 0.65 to 0.90, with a step of 0.025. The perturbation of the parameter in computing the derivative of the system matrix is 1%, which is the same as we used with the computation of the FFD method. Fig. 1 and 2 show the derivative of the magnitude and phase of S21 with respect to d/a at $f = 2.1$ GHz. The results show that the derivatives obtained from the self-adjoint method and the finite-difference method match excellently.

2. Results with the Method of Moments (FEKO [9])

We consider the high-temperature superconducting (HTS) bandpass filter of [10]. This filter is printed on a substrate with relative dielectric constant $\varepsilon_r = 23.425$, height $h = 0.508$ mm and substrate dielectric loss tangent of 0.00003. Design variables are the lengths of the coupled lines and the separations between them, namely, $x = [S_1\ S_2\ S_3\ L_1\ L_2\ L_3]^T$. The length of the input and output line is $L_0 = 1.27$ mm and the lines are of width $W = 0.1778$ mm. It is analyzed at $f = 4.0$ GHz. We compute the self-adjoint sensitivities of the S_{21} magnitude and phase, compared with the finite differences. Fig. 3 shows the derivatives of $|S_{21}|$ with respect to the spacing between the first coupled lines S_1 ($0.5 \le S_1 \le 0.75$ mm) when $[S_2\ S_3\ L_1\ L_2\ L_3]^T = [2.3764\ 2.6634\ 4.7523\ 4.8590\ 4.7490]^T$. Fig. 4

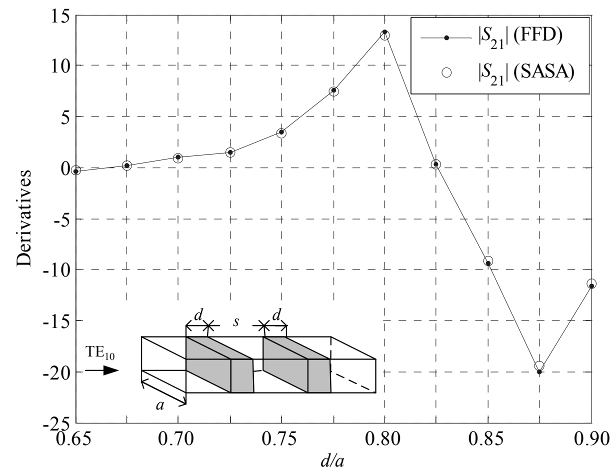

Fig. 1. Derivatives of $|S_{21}|$ with respect to d/a at f=2.1 GHz for the dielectric coupling filter.

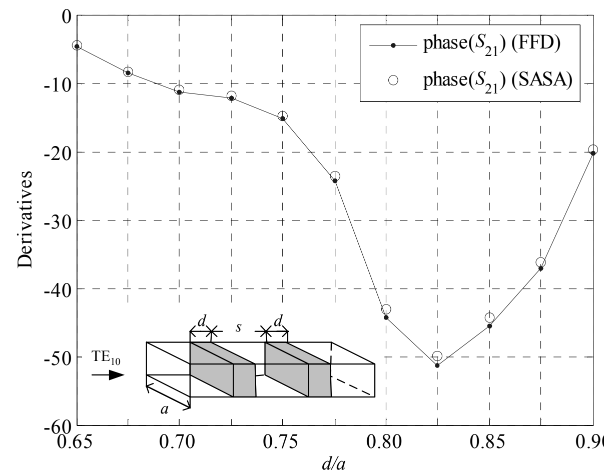

Fig. 2. Derivatives of $\varphi(S_{21})$ with respect to d/a at f=2.1 GHz for the dielectric coupling filter.

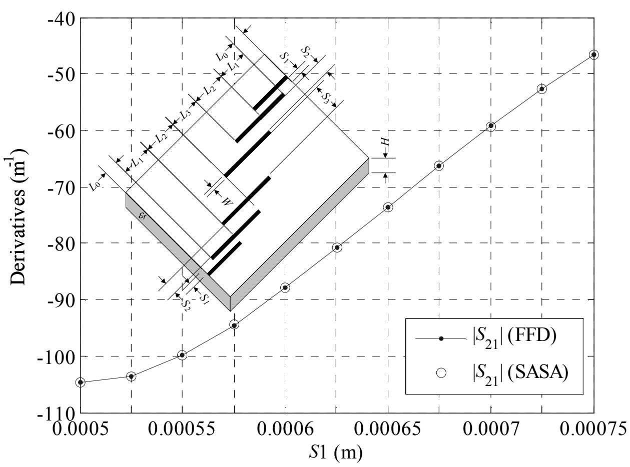

Fig. 3. Derivatives of $|S_{21}|$ with respect to S_1 at f=4.0 GHz for the HTS filter.

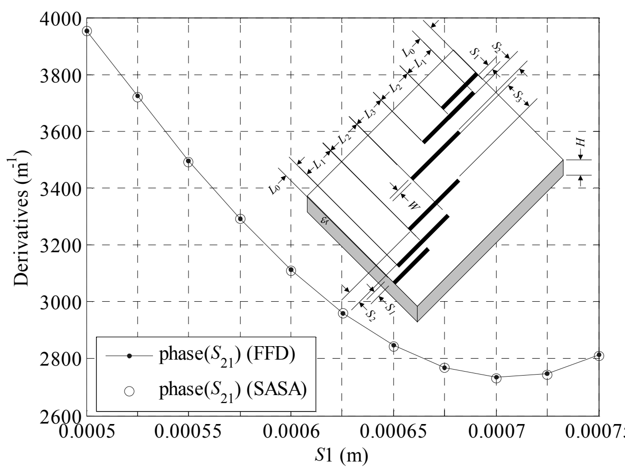

Fig. 4. Derivatives of $\varphi(S_{21})$ with respect to S_1 at f=4.0 GHz for the HTS filter.

shows the derivatives of the respective phase. Again, very good agreement is observed between the self-adjoint derivatives and the respective finite-difference estimates.

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