A Fast Finite-Element-Based Field Optimizer Using Analytically Calculated Gradients

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***Abstract*—A novel and efficient gradient-based optimization technique for the finite-element method (FEM) is described. In contrast to the standard approach in which finite differences are used to determine the gradient of a cost function, the new technique calculates the gradient analytically. This offers many advantages, among which the most prominent ones are: only a single FEM analysis is necessary to find the gradient and no mesh readjustment is required. Thus, computer resources like memory and CPU time are reduced significantly. The analytically calculated gradient is exact and singularities (as in the finite-difference technique) are eliminated.**

***Index Terms*—CAD, finite-element methods, gradient methods, optimization methods, resonance, scattering parameters, simulation, waveguide filters.**

I. Introduction

ACCURATE design of increasingly complex microwave circuits can often be achieved only through sophisticated optimization methods. It is generally accepted that efficient optimization methods are those exploiting not only the values of the cost function, but its gradient and even its Hessian matrix as well. The gradient of the cost function is, most of the time, evaluated by repeated analyses at closely spaced values of the independent variables. Such a process can be prohibitively time consuming when the number of independent variables is large and when the analysis method itself is very general. This applies in particular to the finite-element method (FEM). The generality of the FEM necessitates a large amount of computer memory and CPU time, and it is, thus, not surprising that the FEM has not found widespread use in the optimization of microwave structures since hundreds or even thousands of analysis runs may be required.

To some extend, this problem has been addressed recently by a fully automated space mapping optimization of three-dimensional (3-D) structures [1]. This approach is based on a combination of electromagnetic (EM) simulators (e.g., the commercial 3-D FEM simulator HFFS) and empirical engineering models. The EM simulators generate the so-called fine models (accurate, but computationally slow), which are then mapped onto coarse models (not exact, but computationally fast) using parameter-extraction techniques. The optimization is then performed with the coarse model; thus, significantly reducing computation time. Coarse models can either be coarse-resolution EM or empirical models. The problem with the latter is that, for each specific microwave structure, an empirical model has to be derived. Other techniques that use a combination of Broyden updates and finite differences to accelerate the FEM optimization are described in [2].

For general analysis techniques to offer a viable design alternative to more restricted and albeit much more effective methods, it is necessary to develop ways of extracting from a single analysis more than simply the value of the solution. The mere inclusion of information on the sensitivities of the solution to structural changes in the system, if these are evaluated at minor additional computational cost, will certainly give a new push to the idea of optimization using these general techniques.

In this paper, we propose a method to compute all port sensitivities of a microwave structure from a single analysis using the FEM. Gradients of port parameters such as scattering parameters can be computed analytically from a single analysis and without finite differencing. The advantages of the herein described approach over the traditional finite differences are indeed tremendous, especially for the FEM where using finite differences to evaluate gradients requires not only two separate analyses, but a re-meshing for each independent variable. More specifically, the present approach offers the following features:

1) analytic calculation of gradients of cost and port functions without finite differences;
2) all gradients are computed from a single analysis of the structure regardless of its complexity;
3) it is not even necessary to invert a large matrix; a linear system $[K]\{E\} = \{b\}$ is solved instead;
4) no re-meshing is needed;
5) the gradient values are exact in the sense of the approximate solutions generated by the FEM;
6) finite differences can be optionally used on the matrix $[K]$ and not the solution.

It is worth describing briefly these points one by one. The first point allows a considerable reduction in CPU time. The second point makes it possible to apply the technique to any structure that can be analyzed by the FEM. The third point reduces the overall CPU time since inverting a matrix $[K]$ is an N^3 process, while solving a set $[K]\{E\} = \{b\}$ is an N^2 operation ($[K]$ is a symmetric band matrix in the FEM [3]). By using only one analysis, it is not necessary to readjust the mesh to calculate the gradient. The fifth point emphasizes the robustness of the approach even in the vicinity of strong resonances where the finite-difference approach fails. Finally, the method is flexible enough to allow one to use finite differences on the matrix $[K]$, analyze the structure only once, and yet compute all network

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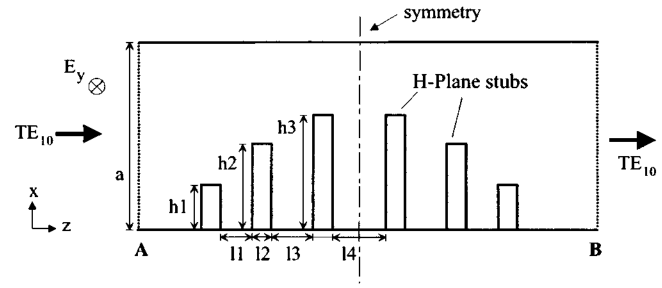

Fig. 1. H-plane iris filter.

sensitivities. Although a somewhat similar idea was proposed in [4], the method was limited to the optimization of permittivities using the FEM in conjunction with the adjoint state vector. In [5], the authors have developed this approach much further for the optimization of microwave structures calculated by the coupled-integral-equations technique (CIET) and, in this paper, the method is expanded to optimize general microwave structures with the FEM.

II. Theory

The key to this new approach is to put the analysis of the structure to be optimized into a scattering problem representation of the form

$$[A]\{x\} = \{b\}. \tag{1}$$

Here, $[A]$ is a $M \times M$ matrix, which depends on the independent variables and represents the structure to be optimized, $\{b\}$ is the excitation, and $\{x\}$ is the response.

The optimization problem consists in determining the optimal values of the independent geometrical variables $a_1, a_2, a_3, \ldots, a_n$ such that the response function is equal to an optimal function x^{opt}. Note that the independent variables appear explicitly in both the matrix $[A]$ as well as in the excitation $\{b\}$ in general. We assume also that the optimization problem consists in minimizing a cost function F, which depends explicitly on the solution $\{x\}$.

To illustrate the procedure, we have chosen a waveguide H-plane iris filter (shown in Fig. 1). The task is to optimize a filter response to given specifications. For that purpose, a suitable cost function has to be found. Generally, the cost function consists of the differences between computed and desired data of the scattering parameters. A possible cost function is given below.

Function $F(a_i)$ has to be minimized during the optimization process

$$F(a_i) = \sum_n W_n \left[|S_{11}(\omega_n, a_i)| - \left| S_{11}^{\text{optimal}}(\omega_n, a_i) \right| \right]^2 \tag{2}$$

where $S_{11}(\omega_n, a_i)$ is the reflection coefficient of the structure, which depends on the frequency as well as the geometric parameters a_i, $i = 1, \ldots, N$.

Here, W_n are constants and ω_n are specified frequencies in the desired band.

For the gradient of the function $F(a_i)$, we take the partial derivatives with respect to the parameters a_i

$$\frac{\partial F}{\partial a_i} = 2 \sum_n W_n \left[|S_{11}(\omega_n, a_i)| - \left| S_{11}^{\text{optimal}}(\omega_n, a_i) \right| \right] \cdot \frac{\partial |S_{11}(\omega_n, a_i)|}{\partial a_i}. \tag{3}$$

The partial derivatives of the absolute value of the reflection coefficient are easily found as

$$\frac{\partial |S_{11}|}{\partial a_i} = \text{Re} \left[\frac{|S_{11}|}{S_{11}} \frac{\partial S_{11}}{\partial a_i} \right]$$

similarly for the transmission coefficient. For clarity of presentation, the distance between the irises in the structure of Fig. 1 are kept constant and only their height is subject to optimization.

In order to calculate the scattering parameters with the FEM, the transmitted and reflected waves are determined at the following reference planes.

- Cutting plane A:

$$E_y = E_y^{\text{inc}} + E_y^{\text{ref}} = E_0 \sin(k_x x) \left[e^{-jk_z z} + S_{11} e^{jk_z z} \right]. \tag{4}$$

- Cutting plane B:

$$E_y = E_y^{\text{trans}} = S_{21} E_0 \sin(k_x x) e^{-jk_z z}. \tag{5}$$

Here, $k_x = \pi/a$, $k_0^2 = k_x^2 + k_z^2$.

For simplicity, we have chosen the two-dimensional (2-D) FEM using scalar interpolation functions and a triangular mesh. It is straightforward to extend the procedure to the 3-D FEM.

The structure in Fig. 1 is assumed to be lossless and the incident fundamental TE_{10}-mode excites only TE_{m0} modes. We are interested in S_{11} and S_{21} of the fundamental mode at the cutting planes A and B. The assumption is that, at these planes, all higher order modes have vanished. The electric field at plane A is obtained from the scalar Helmholtz equation ($\mu_r = 1$)

$$\frac{\partial}{\partial x} \left(\frac{1}{\mu_r} \frac{\partial E_y}{\partial x} \right) + \frac{\partial}{\partial z} \left(\frac{1}{\mu_r} \frac{\partial E_y}{\partial z} \right) + k_0^2 E_y = 0. \tag{6}$$

Considering the boundary conditions (Dirichlet $E_y = 0$ at waveguide walls (electric wall) and Neumann $\partial E_y / \partial n = 0$ at magnetic walls), the electric field satisfies the following relations:

$$\begin{aligned} \frac{\partial E_y}{\partial z} - jk_z E_y &= -jzk_z E_0 \sin(k_x x) \text{ at plane A} \\ \frac{\partial E_y}{\partial z} + jk_z E_y &= 0 \text{ at plane B} \end{aligned} \tag{7}$$

and the scattering parameters we are interested in are found from

$$S_{11} = \frac{E_y(z=0)}{E_0 \sin(k_x x)} - 1 \quad S_{21} = \frac{E_y(z = z_B)}{E_0 \sin(k_x x) e^{-jk_z z_B}} \tag{8}$$

provided the dielectric is lossless and power conservation ($|S_{11}|^2 + |S_{21}|^2 = 1$) holds.

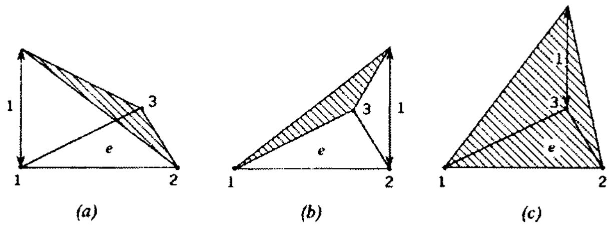

Fig. 2. Linear interpolation functions (a) N_1, (b) N_2, (c) N_3.

The functional associated with (6) is

$$F^e(E_y^e) = \frac{1}{2}\iint_{\Omega_e}\left(\left(\frac{\partial E_y^e}{\partial x}\right)^2 + \left(\frac{\partial E_y^e}{\partial z}\right)^2 - k_0^2 (E_y^e)^2\right) + \int_{\Gamma_A}\left[2jk_z E_0 \sin(k_x x) E_y^e - \frac{jk_z}{2}(E_y^e)^2\right] d\Gamma - \int_{\Gamma_B}\left[\frac{jk_z}{2}(E_y^e)^2\right] d\Gamma. \tag{9}$$

Here, Ω_e is the area of element e, Γ_A is the boundary A, and Γ_B is boundary B. Equation (9) is readily found from the FEM analysis of the computational domain [6].

Discretizing the structure into triangles, the electric field E_y^e inside one triangle e can be expressed as

$$E_y^e(x, z) = \sum_{j=1}^{3} N_j^e(x, z) E_{y,j}^e \tag{10}$$

where $N_j^e(x, z)$ are the interpolation or expansion functions (Fig. 2) given by

$$N_j^e(x, z) = \frac{1}{2\Delta^e}(a_j^e + b_j^e x + c_j^e z), \qquad j = 1, 2, 3$$

with

$$a^e = \begin{pmatrix} z_2^e x_3^e - z_3^e x_2^e \\ z_3^2 x_1^e - z_1^e x_3^e \\ z_1^e x_2^e - z_2^e x_1^e \end{pmatrix}$$

$$b^e = \begin{pmatrix} x_2^e - x_3^e \\ x_3^e - x_1^e \\ x_1^e - x_2^e \end{pmatrix}$$

$$c^e = \begin{pmatrix} z_3^e - z_2^e \\ z_1^2 - z_3^e \\ z_2^e - z_1^e \end{pmatrix}$$

$\Delta^e = (1/2)(b_1^e c_2^e - b_2^e c_1^e)$.

It can be shown that the interpolation functions have the property [6] $N_i^e(x_j^e, z_j^e) = \delta_{ij}$.

With the expansion of E_y^e, we can proceed to formulate the system of equations using either the Ritz or Galerkin methods. The functional for this variational problem is $F(E_y) = \sum_{e=1}^{M} F^e(E_y^e)$, where M is the total number of triangles and e is the element number, with $F^e(E_y^e)$ given in (9). Differentiating this functional with respect to $E_{y,j}^e$ and arranging the results in matrix form, we get

$$\sum_{e=1}^{M}\left[K^e\right]\left\{E_y^e\right\} + \sum_{s=1}^{M_s}\left(\left[K^s\right]\left\{E_y^s\right\} - \left\{b^s\right\}\right) = \{0\}. \tag{11}$$

The following notations are used in this equation:

$$K_{ij}^e = \frac{1}{4\Delta^e}(b_i^e b_j^e + c_i^e c_j^e) - k_0^2 \frac{\Delta^e}{12}(1 + \delta_{ij})$$
$$K_{ij}^{s=\Gamma_A} = -jk_z \frac{l^s}{6}(1 + \delta_{ij})$$
$$K_{ij}^{s=\Gamma_B} = jk_z \frac{l^s}{6}(1 + \delta_{ij})$$
$$b_i^{s=\Gamma_A} = -2jk_z E_0 \sin(k_x x)\frac{l_s}{2}.$$

Equation (11) index: s: edge number (edges on A or B), e: triangle number, l_s: edge length.

$K_{ij}^e \Rightarrow K_{n(i,e),n(j,e)}$, $K_{ij}^s \Rightarrow K_{n(i,s),n(j,s)}$ (i, j are local node numbers of element e; $n(i, e)$, $n(j, e)$ are the corresponding global node numbers) and similar with the nodes on the boundaries A and B to get the system of equations typical for the FEM as follows:

$$[K]\left\{E_y\right\} = \{b\}. \tag{12}$$

The coefficients E_y are not only the solutions of the system, but also the values of the electric field in the y-direction for all nodes in the mesh. The reflection and transmission coefficients can now be calculated from (8).

III. Analytical Gradient Evaluation

Taking the derivatives of (12) yields

$$[K]\frac{\partial}{\partial h_i}\left\{E_y\right\} = \frac{\partial}{\partial h_i}\{b\} - \left(\frac{\partial}{\partial h_i}[K]\right)\left\{E_y\right\}. \tag{13}$$

According to (8), S_{11} is a function of E_y at plane A and, therefore, the gradients of S_{11} are functions of the gradients of E_y as follows:

$$\frac{\partial S_{11}}{\partial h_i} = \frac{1}{E_0 \sin(k_x x)}\frac{\partial E_y(z=0)}{\partial h_i}. \tag{14}$$

One way to solve (14) is the following:

$$\frac{\partial S_{11}}{\partial h_i} = \frac{1}{E_0 \sin(k_x x)}[K]^{-1}\left(\frac{\partial}{\partial h_i}\{b\} - \left(\frac{\partial}{\partial h_i}[K]\right)\left\{E_y\right\}\right). \tag{15}$$

However, this requires a matrix inversion and, thus, is not the best option. A better way avoiding matrix inversions is to solve (13) directly for $(\partial/\partial h_i)\{E_y\}$. $[K]$ and $\{E_y\}$ are known from the calculation of S_{11}. The gradient of the excitation $(\partial/\partial h_i)\{b\}$ is zero because there are no structural changes at the excitation plane A. Hence, one only needs to calculate the derivatives of the matrix elements, which are functions of h_i. To illustrate the procedure, we limit ourselves to find the optimum heights of the irises in the waveguide filter shown in Fig. 1. The thickness of the irises is kept constant (1-mm standard metallization thickness).

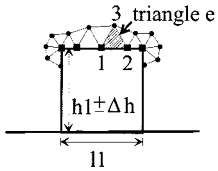

Fig. 3. Single H-plane iris with triangular mesh.

Fig. 3 shows a single iris of the filter partly discretized by a triangular mesh. By changing the height h_1, the nodes marked with a square are moving up or down. The nodes marked with a circle stay fixed. All triangles shown in the figure will change their area. The matrix elements of $[K]$ are functions of the triangle areas and coordinates of the nodes. If we change the heights of the iris (Fig. 3), we change the x-coordinates of the nodes residing on the stubs. Therefore, the b's and the triangle area will change according to $x_i \rightarrow x_i(h/h_1)$. A closer look at K_{ij}^e is quite revealing as follows:

$$K_{ij}^e = \frac{1}{4\Delta^e}\left(b_i^e b_j^e + c_i^e c_j^e\right) - k_0^2 \frac{\Delta^e}{12}\left(1 + \delta_{ij}\right). \qquad (16)$$

For triangle e (hatched in Fig. 3) with nodes 1 and 2 on the moving edge, one obtains

$$b^e = \begin{pmatrix} x_2^e \frac{h}{h_1} - x_3^e \\ x_3^e - x_1^e \frac{h}{h_1} \\ x_1^e \frac{h}{h_1} - x_2^e \frac{h}{h_1} \end{pmatrix}$$

and

$$\Delta^e = \frac{1}{2}\begin{vmatrix} 1 & z_1^e & x_1^e \frac{h}{h_1} \\ 1 & z_2^e & x_2^e \frac{h}{h_1} \\ 1 & z_3^e & x_3^e \end{vmatrix}.$$

It follows for the partial derivatives of K_{11}^e, height $h = h_1$, e.g.,

$$\frac{\partial K_{11}^e}{\partial h_1} = \frac{8\Delta^e b_1^e y_2^e - 2\left(b_1^e b_1^e + c_1^e c_1^e\right)\left(x_2^e c_2^e - x_1^e c_1^e\right)}{h_1(4\Delta^e)^2} - \frac{k_0^2}{12}\left(x_2^e c_2^e - x_1^e c_1^e\right).$$

For all other elements $\partial K_{ij}^e/\partial h$, the procedure is similar. If the gradient with respect to all variables is evaluated, a standard gradient optimization routine can be utilized for further processing.

In summary, the procedure is as follows.

1) Substitute the values of the x-coordinates of the nodes marked with square $x_i \rightarrow x_i(h_1/x_i)$ or $x_i \rightarrow x_i + h$.
2) Do the same for the other irises.
3) Take the derivatives of all matrix elements that are related to the nodes marked with a square or a circle with respect to h_1, h_2, and h_3.
4) Put the results in matrices $\partial[K]/\partial h_i$.
5) Solve (13) for
$$\frac{\partial\{E_y\}}{\partial h_i} \rightarrow \frac{\partial S_{11}}{\partial h_i} \rightarrow \frac{\partial F}{\partial h_i}.$$
6) Supply the optimization routine with analytically calculated gradients of $\partial F/\partial h_i$.

Although the substitution of a parameter as described under 1) is only applicable for moving or stretching a stub or a rectangle, respectively, more general structures consisting of a mixture of rectangles, cylinders, circles etc. can be optimized as well. A more general way than the one shown here to describe arbitrary geometrical structures as functions of user-defined parameters can be found in [7]. By using this method, the geometrical objects and, hence, the nodes or vertices of the mesh triangles residing on those objects that are subject to optimization (structural changes), are given as mathematical formulations. These formulations include the optimization parameters. It is then straightforward to proceed as illustrated in 1)–6) to calculate the gradients, which can then be used for automated EM optimization.

IV. Discussion

The actual implementation of the technique can further reduce the numerical effort. The gist of the approach is the following identity, which follows from (12) by the following differentiation:

$$[K]\frac{\partial}{\partial h_i}\left\{E_y\right\} + \left(\frac{\partial}{\partial h_i}[K]\right)\left\{E_y\right\} = \frac{\partial}{\partial h_i}\{b\}.$$

The quantity of interest is the gradient of the solution $(\partial/\partial h_i)\{E_y\}$. Since both $\{b\}$ and $\{E_y\}$ are column vectors, it is advantageous to avoid inverting the matrices involved and, instead, solve for these column vectors. This simple scheme reduces the CPU time by a factor of three and is described as follows.

1) Solve the linear set $[K]\{E_y\} = \{b\}$ without first inverting the matrix $[K]$ (numerical recipes [8]).
2) Compute partial derivatives $(\partial/\partial h_i)\{K\}$.
3) Substitute those in
$$[K]\frac{\partial}{\partial h_i}\left\{E_y\right\} = \frac{\partial}{\partial h_i}\{b\} - \left(\frac{\partial}{\partial h_i}[K]\right)\left\{E_y\right\}.$$
4) Solve this last equation for $(\partial/\partial h_i)\{E_y\}$ again without inverting the matrix $[K]$.

Point 4) can be carried out by using an already processed matrix $[K]$ from point 1). (e.g., LU decomposition).

V. Results

Fig. 4 shows the results of the optimization of the H-plane iris filter (Fig. 1). The size of the standard waveguide (WR75) is $a \times b = 19.05$ mm × 9.525 mm. The distances between the irises (thickness $l_2 = 1$ mm) have been kept fixed: $l_1 = 21.6580$ mm, $l_3 = 23.6964$ mm, $l_4 = 23.8727$ mm. The starting values for the variable heights have been chosen as $h_1 = 6.8$ mm, $h_2 = 10.2$ mm, and $h_3 = 11.3$ mm. For the gradient optimization process, we have utilized the Matlab routine "constr" and a triangular mesh with approximately 5500 triangles, 3000 nodes, and 50 frequency points. The routine converged after 19 iterations and delivered the optimal heights $h_1 = 7.17485$ mm, $h_2 = 10.4285$ mm, and $h_3 = 11.0367$ mm. The results for S_{11} for both start and optimized parameters are shown in Fig. 4. S_{21}

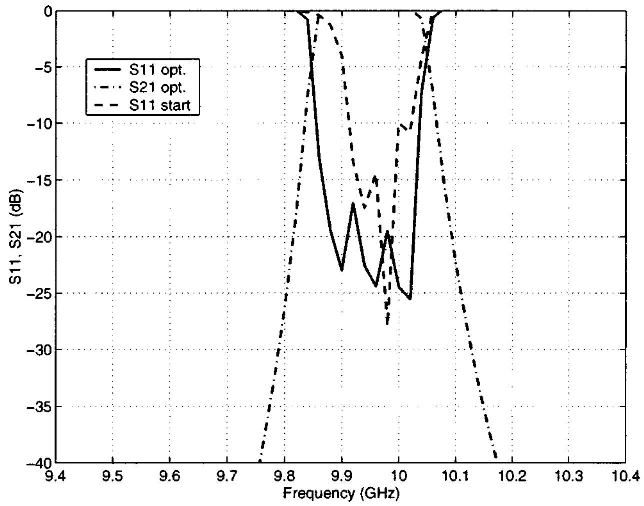

Fig. 4. Optimization results of the H-plane iris filter.

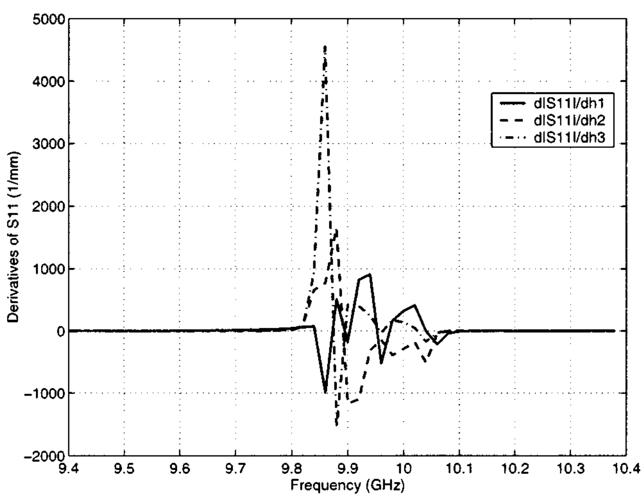

Fig. 5. Derivatives of S_{11} of the H-plane iris filter.

for the optimized values is also displayed. The optimized return loss in the passband is better than 15 dB.

In Fig. 5, the derivatives of S_{11} with respect to the iris heights are shown. It can be seen that the investigated filter is very sensitive to structural changes and large values for the derivatives can occur. It is obvious that evaluating the derivatives with finite differences can give errors especially near the sharp peaks.

Another filter that has been investigated is shown in Fig. 6. The variables are the openings of the inductive irises h_1 and h_2, respectively. The dimensions of the filter are given in the figure. The FEM approach is the same as for the asymmetric H-plane iris filter (Fig. 1).

Fig. 7 shows the result of the optimization of the H-plane filter (Fig. 6). Although with a filter synthesis program better starting values could have been obtained, the intention was to go far away from the goal values to show the validity of this method. For the analysis, a triangular mesh with about 2000 triangles and 1100 nodes and 100 frequency points have been used to guarantee sufficient accuracy. The optimization process converged after 23 iterations. The same structure has been investigated in [9] using an equivalent-circuit model and the mode-

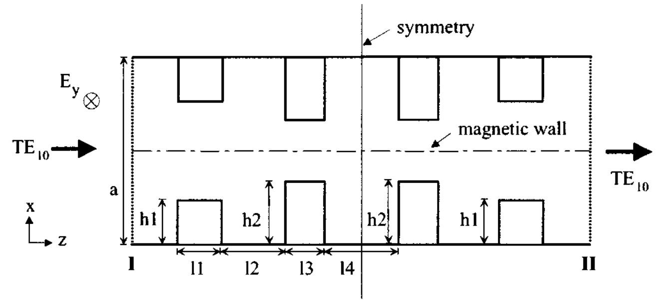

Fig. 6. Bandpass filter for the Ka-band: $a = 7.10$ mm, $l_1 = 1.45$ mm, $l_2 = 4.15$ mm, $l_3 = 1.10$ mm, $l_4 = 4.70$ mm, $h_1 = 1.75$ mm, and $h_2 = 2.35$ mm. h_1, h_2 are variables.

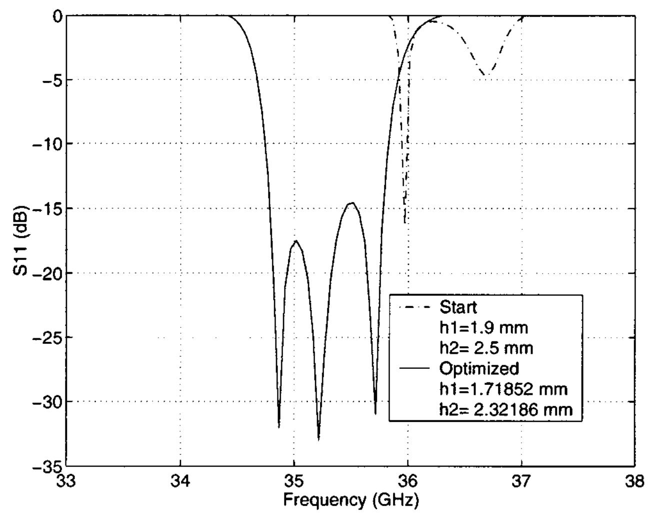

Fig. 7. Optimization results.

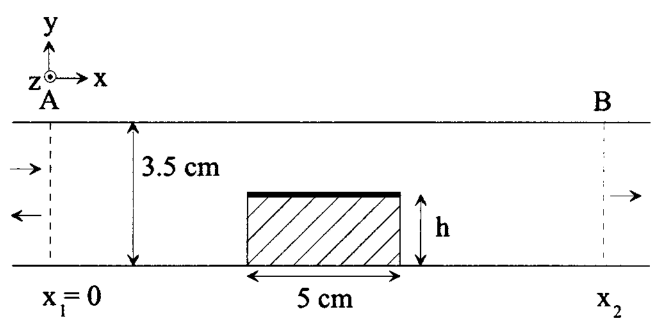

Fig. 8. Parallel-plate waveguide with dielectric insert ($\epsilon_r = 4$), infinitely long in the z-direction.

matching technique with edge condition, and good agreement was found.

Dielectrically loaded waveguide structures can also be optimized with the 2-D FEM optimizer. The structure, a parallel-plate waveguide with a lossless dielectric insert, is shown in Fig. 8. The FEM analysis is similar to the one explained above, except that now the H-field in the z-direction (H_z) was used as a quantity of interest. The reflection and transmission coefficient $S_{11}(\omega, h)$ and $S_{21}(\omega, h)$ and the gradient of $S_{11}(\omega, h)$ with respect to $h(\partial S_{11}(\omega, h)/\partial h)$ are functions of H_z. The mesh used for this structure is shown in Fig. 9.

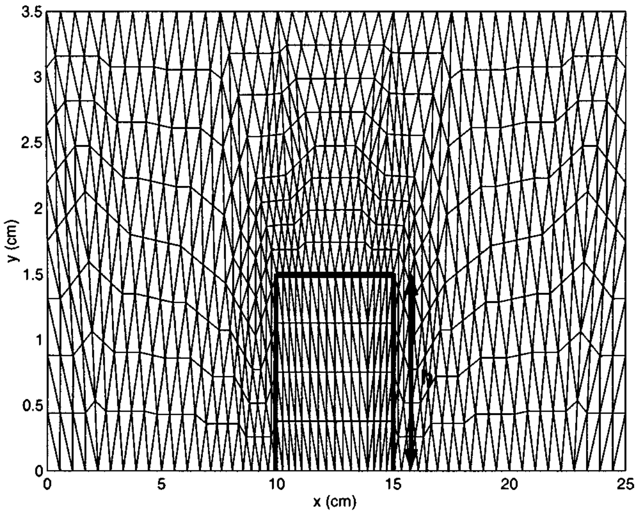

Fig. 9. Mesh setting: triangular mesh with 1088 elements and 601 nodes.

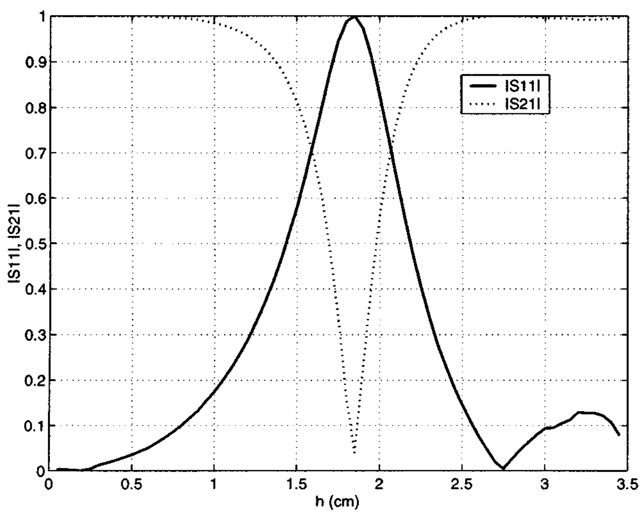

Fig. 10. Reflection and transmission coefficient versus height h (in centimeters).

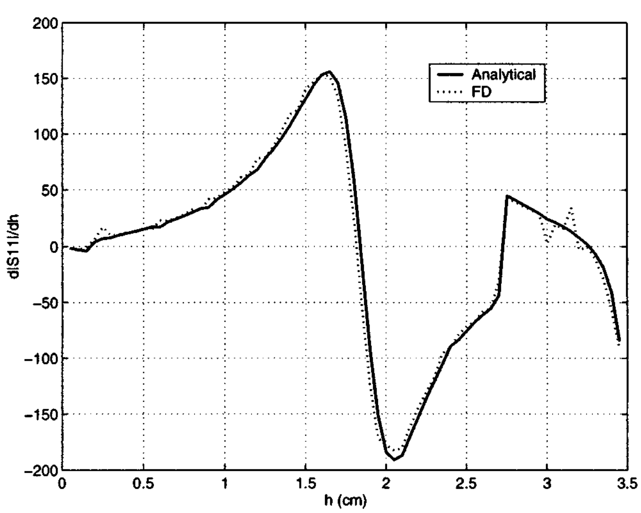

Fig. 11. Derivatives of $|S_{11}|$ with respect to h versus height h (in centimeters). Finite-difference calculated with increment $\Delta h = 0.05$ cm.

The transmission and reflection coefficient of the structure is calculated at $f = 3$ GHz and is given in Fig. 10. Finally, the analytically evaluated gradient is compared to the gradient evaluated with finite differences. This is illustrated in Fig. 11. The finite-difference gradient is calculated by varying the height of the stub by the increment $\Delta h = 0.05$ cm. A new mesh is then put onto the structure and the reflection coefficient is calculated again. The difference between the calculated reflection coefficients divided by the increment Δh gives the finite-difference gradient. The analytical gradient is calculated by the technique proposed in this paper. Only the nodes that touch the dimension that is changing have to be taken into account (see Fig. 3). Good agreement can again be observed between the analytically calculated gradient and the one obtained through finite differencing.

VI. Conclusions

We have developed a method for analytically calculating the gradient of a cost function in conjunction with a general field solver. The method only requires that the problem be formulated in terms of a general inhomogeneous matrix equation such as generated by the FEM. All partial derivatives are determined from a single analysis of the structure, no matrix inversion is required, and no re-meshing of the FEM grid is needed. Numerical results show excellent agreement between the current approach and the finite-difference method when small enough increments are used. Results of the optimization show the validity of the whole process.

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