Gradient-Based Optimization of Filters Using FDTD Software

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***Abstract*—This letter discusses gradient optimization of bandpass filters using electromagnetic simulation software based on the finite difference-time domain algorithm. It is shown that even high-Q-factor circuits can be optimized in acceptable time if robust digital signal processing techniques that take into account signal dynamics are used to predict the frequency behavior of a structure from relatively short sample sequences.**

***Index Terms*—Filters, finite difference-time domain (FDTD), optimization, signal processing.**

I. INTRODUCTION

INCREASING performance of workstations and progress in computational electromagnetics are beginning to change the way in which microwave circuits are designed. Nowadays, full wave analysis is often used in the optimization loop. Most commercial microwave CAD suites offer some sort of electromagnetic-based optimization. One area where successful full-wave design by optimization has been demonstrated are cavity bandpass filters [1], [4], [5]. One of the most important factors that one has to take into account while selecting a numerical tool to be used for the analysis is the speed of computations. For these reasons, time domain methods seem to be inferior to frequency domain approaches when it comes to the analysis and optimization of bandpass filters. Indeed, while frequency domain techniques such as finite element [4], mode matching [2], and finite differences [7], have all been used so far for filter design by optimization, the application of time domain methods has only been reported for full-wave optimization of broadband components [10], [6], such as transitions or waveguide bends. The reason for this is that time domain techniques require many iterations and, hence, long simulation times to characterize circuits with high Q-factors. On the other hand, techniques such as finite-difference time-domain (FDTD) and TLM do not involve solution of a system of equations and consequently can handle larger geometries. Additionally, commercial state-of-the-art implementations of time domain techniques are versatile, allow for arbitrary three-dimensional (3-D) geometries, and can take into account conductor and dielectric losses, nonhomogeneous materials and technical limitations of manufacturing process. In this letter, we show that even circuits with high quality factors can be optimized in acceptable time if a time domain electromagnetic simulator is enhanced with a robust digital signal processing method that takes into account the signal's dynamics, time step size, and automatically creates waveform models which accurately predict the frequency behavior of a structure from relatively short sample sequences.

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II. AUTOMATED SIGNAL PROCESSING

The design process of filters involves two steps at which EM simulation can be used. After a lumped model has been created, EM solvers can be used to analyze and optimize isolated circuits and find initial values (such as couplings or resonator lengths). Next, full-wave modeling tools can be employed to fine tune the overall filter response taking into account all interactions, presence of higher order modes, etc. Both steps involve the analysis of circuits with different physical dimensions and loaded Q-factors. These two aspects greatly influence the performance of the time domain simulators. First, time domain solvers use nonuniform mesh and the time step size is proportional to the smallest mesh size. Changing the circuit dimensions requires remeshing and this implies that each analysis can be performed with a different time step size and hence more iterations are required to reach the steady state. This problem is particularly important when gradient-based optimization techniques are used. Numerical computation of gradients involves small changes of dimensions and, thus, the time step may change significantly. Moreover, the optimization procedure creates circuits with different Q-factors. The simulation can be terminated earlier for structures with low Q, but some combinations of dimensions may lead to structures with high Q-factors which require much more time steps. Keeping these limitations in mind, we developed a robust digital signal processing procedure [11] and [12], which automatically creates high-quality low-order signal models and takes into account the bandwidth, Q-factor, and time step size. The procedure is based on the generalized pencil of function (GPOF) method [9]. The GPOF method constructs the model of a signal in the form of a superposition of P damped sinusoids, where P is a model order. Its successful application requires the specification of several key model parameters that have to be determined automatically during the optimization process. The most important issues that have to be resolved include the problem of the number of initial samples of the FDTD record to be discarded, the length of the time sequence required for model construction, preprocessing of samples that reduces the computational effort and improves numerical conditioning and finally the model order selection, and the computation of the frequency responsed [11] and [12].

A. Accounting for Transients, Signal Dynamics, and Time Step Size

The model describes slow-decaying signal components, so the early time response should be discarded. Building the model prematurely may entail problems with automatic model order selection and lead to unstable models. Also, waveforms coming out of circuits with lower Q-factors decay faster, and, hence, the model can be created earlier. Both the number of samples to be discarded and the length of time sequence required for building a model can easily be selected by monitoring the energy of signals passing thought the ports of the circuit.

The energy is calculated for each port separately using the moving average filter [14]. No model is created until the moving average energy starts decreasing. All time samples calculated up to this moment are discarded, but the FDTD simulation continues until the normalized moving average energy in all ports drops to certain low value. Application of the described approach guarantees that the signal used for model building is not contaminated with strongly damped transients, and its length is well adapted to the signal dynamics.

Next, the samples are preprocessed. The signals obtained from the FDTD simulations are highly oversampled and cannot directly be used for model building. Therefore, they are decimated by the ratio of Nyquist frequency $f_n = 1/2\,dt$, where dt is FDTD time step, the upper frequency ($f_{\max}$) specified for each circuit. The decimation technique depends on the spectrum of the excitation. It is advisable to use the excitation signals with bandwidths slightly greater than the passband of the filter being designed. If this is the case, the decimation involves simply throwing away redundant samples, as no aliasing takes place. All decimated samples may be used as data for GPOF. If the excitation spectrum significantly exceeds $f_{\max}$, then desampling should be preceded by passing a signal through a low pass filter and followed by discarding last few samples from the desampled sequence. If this is not done, the desampled data is distorted by the transients generated by the filter itself, and low quality models are obtained.

B. Construction of the Model and Calculation of Frequency Response

Desampled signals, free from initial transients and transients due to filtering, are used to create a model. First, the model order is selected automatically by simultaneously using two common statistics for model order selection, namely the Akaike information criterion (AIC) [14] and the minimum description length (MDL) [14]. We have found out that it is a more reliable approach than using the criterion based on singular values advocated in [13]. Models of low order are created by zeroing all amplitudes of the model below 10^{-4} and the amplitudes of the sinusoidal terms corresponding to the frequencies outside the bound of interest. Both operations considerably improve the efficiency and consistency of the model order selection.

Once the models have been created, the frequency response is calculating by summing up the discrete Fourier transform of the discarded samples, computed numerically, and the Fourier transform of the model evaluated analytically.

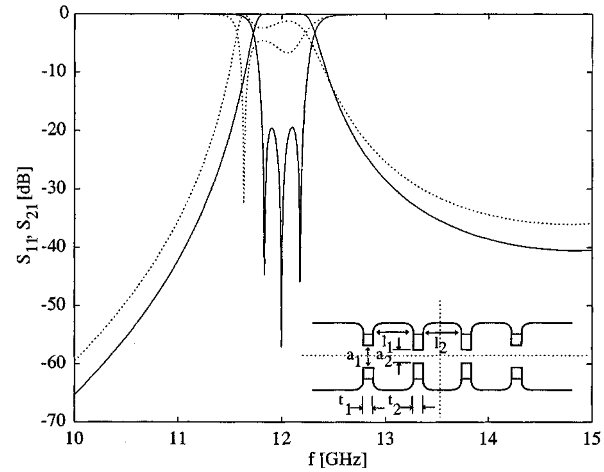

Fig. 1. Scattering parameters of a three-resonator H-plane filter after optimization (—) and before optimization ($\cdots$). (WR-75 waveguide, all dimensions in millimeters: $a = 19.05$, $b = 9.525$, radius of rounded corners $r = 1.5$, $t_1 = 1.73$, $t_2 = 1.93$ $a_1 = 9.52$, $a_2 = 6.62$, $l_1 = 13.42$, and $l_2 = 14.71$).

III. Examples of Design

The signal processing technique described in the previous section was implemented as a procedure linked to a commercial FDTD solver QuickWave 3-D [15], and in this letter, we show its application to fine tuning of entire filter structures. The optimization was performed using the SQP technique available in the Matlab Optimization Toolbox [16]. This is a gradient-based method where gradients can be computed numerically. The cost function used in our computations is that of Amari [8]

$$E = \sum_{i=1}^{N} |S_{11}(\omega_{zi})|^2 + \sum_{i=1}^{P} |S_{21}(\omega_{pi})|^2 + \left(|S_{11}(\omega = -1)| - \frac{\varepsilon}{\sqrt{1+\varepsilon^2}}\right)^2 + \left(|S_{11}(\omega = 1)| - \frac{\varepsilon}{\sqrt{1+\varepsilon^2}}\right)^2 \quad (1)$$

where ε is a constant related to the passband return loss, and ω_{zi} and ω_{pi} are zeros and poles of the filtering function. There are N zeros and P poles.

As a first example, the three-resonator H-plane filter with the return loss -20 dB, band width of 400 MHz, and center frequency at 12 GHz was optimized. The filter geometry and optimized dimensions are shown in Fig. 1, and so are the initial and final characteristics. In this case, six independent variables were optimized simultaneously. The number of function evaluation was 220, including the numerically computed gradients. The total time of the optimization, carried out on a PC-equipped with an AMD 800-MHz processor, was about an hour. The mesh size used in analysis of the circuit with initial dimensions was $103 \times 21 \times 5$.

Next, a filter with the same geometry as a previous one, but with different electrical specifications, namely the return loss equals -30 dB, band width 450 MHz, and center frequency 12 GHz, was optimized (Fig. 2). The same initial guess was

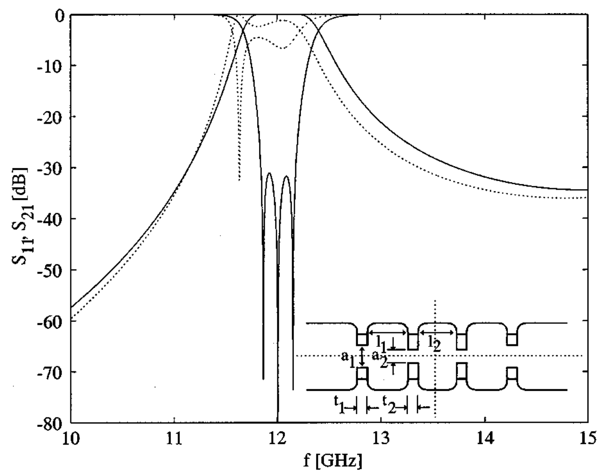

Fig. 2. Scattering parameters of a three-resonator H-plane filter after optimization (—) and before optimization ($\cdots$). (WR-75 waveguide, all dimensions in millimeters: $a = 19.05$, $b = 9.525$, radius of rounded corners $r = 1.5$, $t_1 = t_2 = 1.6$, $a_1 = 10.07$, $a_2 = 6.82$, $l_1 = 13.01$, and $l_2 = 14.53$).

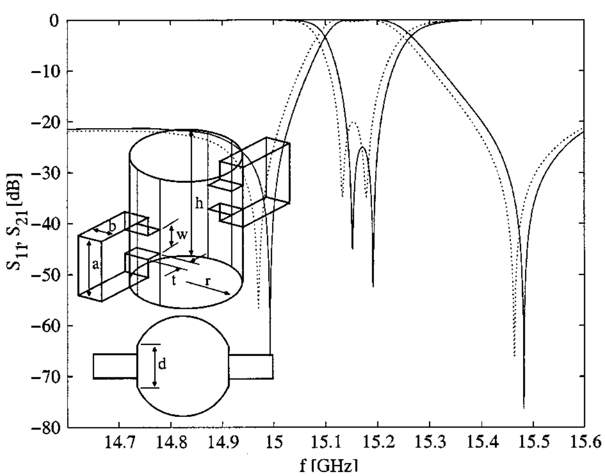

Fig. 3. Scattering parameters of a dual-mode cylindrical cavity filter after optimization (—) and before optimization ($\cdots$). (WR-62 waveguide, all dimensions in millimeters: $a = 15.8$, $b = 7.9$, $r = 12.58$, $h = 32.848$, $w = 8.0$, $d = 8.489$, and $t = 2.4$).

used as in the first example, and, again, six independent variables were optimized in each cycle of the optimization procedure. The number of cost function devaluation was 240. The whole optimization lasted about 1 h 10 min. The initial mesh size was 103 × 21 × 5.

Finally, a detuned dual-mode cylindrical cavity filter, proposed in [3], was optimized. Fig. 3 shows the initial characteristics and the characteristics after tuning by optimization. The number of goal function evaluations was 140. This time, five independent variables were optimized simultaneously, and due to fine meshing (122 × 52 × 66) the total optimization time was about 24 h.

IV. Conclusion

We have demonstrated the optimization of bandpass filters by means of a general purpose time domain electromagnetic solver. The computation times were found to be at an acceptable level owing to the application of a signal processing technique capable of automatically creating models of waveforms of different bandwidth, dynamics and sampling rate.

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