Efficient Computation of Resonant Frequencies and Quality Factors of Cavities via a Combination of the Finite-Difference Time-Domain Technique and the Padé Approximation

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***Abstract*—An efficient method for analyzing cavity structures by using the fast Fourier transform (FFT)/Padé technique, in combination with the finite-difference time-domain method, is presented. Without sacrificing the accuracy of the results, this new method significantly reduces the computational time compared to that needed where the conventional FFT algorithm is used. The usefulness of this approach is demonstrated by modeling a lossy cavity and computing its resonant frequencies as well as Q.**

***Index Terms*— Cavity, fast Fourier transformation, finite-difference time-domain technique, Padé approximation, quality factor, resonant frequency.**

I. Introduction

ACCURATE analysis of the resonant frequencies of cavity resonators is an important field of study since such cavities are used in many microwave applications, e.g., filter and oscillator designs. In most practical applications, the cavity is part of a complex structure that normally includes tuning mechanism and coupling with external circuits, and is only amenable to analysis by using a numerical technique. The finite-difference time-domain (FDTD) technique has been employed in the past for the characterization of various types of cavity resonators [1]. The advantage of the FDTD technique over the frequency domain methods, e.g., the method of moments (MoM) or the finite-element method (FEM), is that the resonant frequencies of all of the modes can be calculated in a single simulation by using the time domain scheme, rather than by sweeping the frequency to capture these modes.

To obtain the resonant frequencies and the quality factors from the FDTD, we must transform the temporal response of the FDTD simulation to the frequency domain, say, by using the fast Fourier transform (FFT). The FFT, however, requires a large number of time samples to calculate the resonant frequency and quality factor with reasonable accuracy and resolution, and this translates to a relatively long computational time.

Several procedures have been proposed in the literature to alleviate the above limitation of the FFT approach. Two commonly employed techniques are the Prony's method [2] and the generalized pencil-of-function [3] technique that eliminates the need for FFT by representing the time signature as a sum of exponents. Although both of these methods have advantages over the FFT in terms of the reduction in the computation time, the accuracy of these results is sensitive to the sampling conditions.

In this letter, we propose to use the Padé approximation [4] in conjunction with the FFT as an alternative to the above two schemes. This new technique is capable of calculating the resonant frequency as well as quality factor from a smaller time window, reducing the computational time significantly in the process.

II. Theory

We can derive the resonant frequencies from the local maxima of the response by carrying out an FFT of the FDTD output, and compute the quality factor by using $Q = f_0/\Delta f$, where Δf is the 3-dB bandwidth and f_0 is the resonant frequency. As pointed out earlier, the inherent limitation of the FFT approach is its inadequacy in frequency resolution, which is reciprocal to the product of total number of iterations and the time step size. Thus, to achieve a reasonably good resolution it is necessary to run the simulation for a sufficiently long time.

To overcome the limitations of FFT method alluded to above, we employ the Padé approximation in conjunction with the FFT as a two-step process. First, we apply the FFT on the time-domain data to obtain the spectral response. We then process this data further by using the Padé approximation to improve the accuracy of the frequency response. The above response can be represented as a sum of pole series

$$P(\omega) = P_p(\omega) + P_{np}(\omega) \tag{1}$$

where $P(\omega)$ is a complex vector-valued function of ω [i.e., $P(\omega) \in C^n$], representing one of the six electromagnetic components. The first term in the right-hand side of (1), viz., $P_p(\omega)$, contains all the pole of $P(\omega)$, whereas the second term, $P_{np}(\omega)$, represents the remainder. The Padé approximation [4] constitutes expressing $P_p(\omega)$ in a rational function as

$$P(\omega) = \frac{Q_N(\omega)}{D_M(\omega)} \tag{2}$$

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where the numerator and denominator polynomials $Q_N(\omega)$ and $D_M(\omega)$ are given by

$$Q_N(\omega) = \sum_{i=0}^{N} \alpha_i \omega^i$$

and

$$D_M(\omega) = \sum_{i=0}^{M} \beta_i \omega^i. \tag{3}$$

Next, we obtain the unknown coefficients α's and β's from the FFT output of the FDTD response. We rewrite (2) as

$$P(\omega_j) \cdot D_M(\omega_j) = Q_N(\omega_j), \qquad j = 0, \cdots, S-1. \tag{4}$$

There are $N + M + 2$ unknown coefficients in the above equation. Hence, an additional condition is required to render it inhomogeneous and we obtain it by setting β_0 equal to unity. Then (4) can be rewritten as

$$P(\omega_j) \cdot \sum_{i=1}^{M} \beta_i \omega_j^i - \sum_{i=0} \alpha_i \omega_j^i = -P(\omega_j), \qquad j = 0, \cdots, S-1. \tag{5}$$

Equation (5) implies that the unknown coefficients of the Padé approximation can be obtained from a system of linear equations and the total number of data samples (FFT output data points) required is $S \geq M + N + 1$. Since the matrix coefficients are now products of a sampled data and some power of the frequency, the dynamic range of the matrix elements is very large for large M's and N's. One way to avoid this problem is to scale the frequency, such that it is near unity. A typical scaling function is as follows:

$$\omega_s = \frac{2\omega - (\omega_{\max} - \omega_{\min})}{(\omega_{\max} + \omega_{\min})} \tag{6}$$

where $\omega_{\max}$ and $\omega_{\min}$ are the maximum and minimum angular frequency of the samples used. Once the coefficients are known, it is straightforward to interpolate the sampled date to obtain the desired resolution. In the application described in this paper, N is chosen to equal M—known as the diagonal Padé approximation—which requires $2N + 1$ data samples.

III. Numerical Results

To test the algorithm, we have studied a rectangular cavity with lossless walls, filled with a slightly lossy medium whose conductivity is 5.1617e-4 s/m. The length, height, and width of the cavity are 2.286, 1.016, and 2.286 mm, respectively, and the corresponding spatial discretizations are 0.057, 0.058, and 0.057 mm. Fig. 1 shows the percentage error in the computed resonant frequency and Q-factor for the TE_{101} mode, as a function of the number of time iterations. For the FFT/Padé combined approach, 13 data samples were used and the number of interpolated outputs were 2700. From the figure it is evident that, for the same number of time iterations, the error in the resonant frequency is nearly ten times less for the FFT/Padé combined technique relative to that of the regular FFT approach. The Q-factor is plotted only for the FFT/Padé approach, because the frequency resolution for the regular FFT

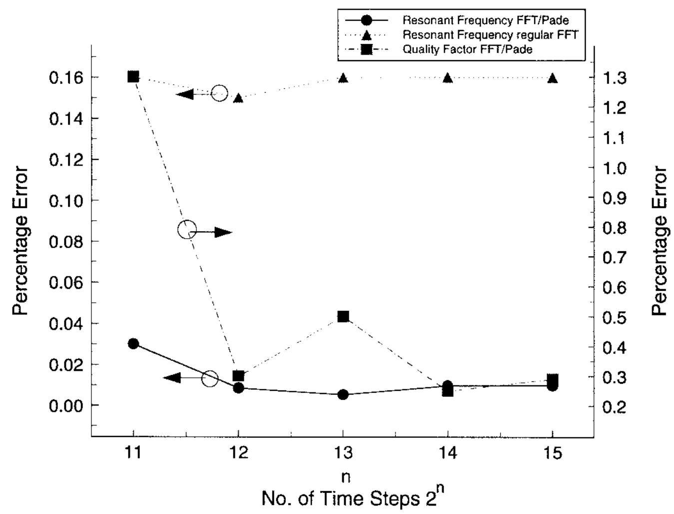

Fig. 1. Percentage error in computed resonant frequency and quality factor of rectangular cavity, for TE_{101} mode, as a function of the number of time iterations.

method is not sufficient enough to compute the Q-factor, even with 2^{15} time iterations.

Next, we examine the effect of number of data samples used in Padé approximation on the accuracy of the results for a fixed number of time iterations, viz., 4096. We can see from Fig. 2, that although the percentage error in the Q-factor increases when the number of data samples is less than seven, its effect on the accuracy of resonant frequency is insignificant. From the above two observations it can be concluded that the FFT/Padé technique is not very sensitive to the choice of the input parameters. Table I show the percentage errors in the resonant frequencies and the Q-factors for the first few dominant modes, computed by using the FFT/Padé technique and the conventional FFT method. For the FFT/Padé approach, 4096 time iterations were used with 13 input samples and the interpolated output samples were 2700. For the same number of time iterations, the improved accuracy of the present method over the regular FFT approach is apparent from Table I. It was found that in most cases the new approach yields more accurate results compared to that of the conventional FFT approach using 32 768 time iterations. Except for one particular mode, the error in the Q-factor is less than 1.5% for the present method. Fig. 3 shows the normalized frequency response calculated by using the conventional FFT as well as by the new technique, with 1024 time iterations. The normalization is carried out independently for the two curves to enhance the clarity of the graph. From the plot it is evident that the conventional FFT is unable to resolve two resonance when they are close to each other due to its resolution limitations. But, from the same data, the new method can easily extract the correct resonant frequencies with errors less than 2%.

IV. Conclusion

In this letter we have presented the combined FFT/Padé approach to accurately calculate the resonant frequency and quality factor of resonant structure. This new method reduces

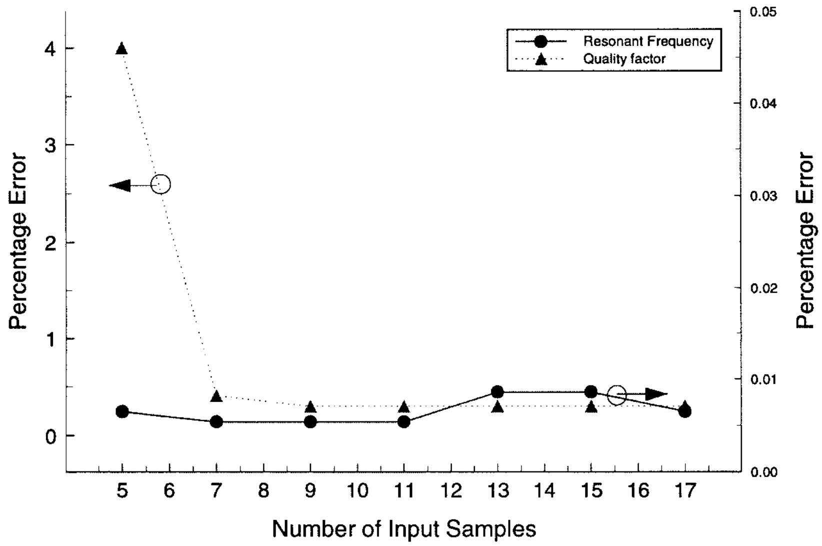

Fig. 2. Percentage error in computed resonant frequency and quality factor of rectangular cavity for TE_{101} mode, as a function of the number of input data samples for Padé approximation for 4096 time iterations.

TABLE I
COMPARISON OF THE PERCENTAGE ERRORS IN RESONANT FREQUENCIES AND QUALITY FACTORS OF FIRST FEW DOMINANT MODES OF A RECTANGULAR CAVITY COMPUTED VIA THE FFT/PADÉ AND THE CONVENTIONAL FFT METHODS FOR DIFFERENT TIME STEPS

Analytical		FFT/Padé (2^{12} time steps)		Conventional FFT Resonant Frequency	
Resonant Frequency (GHz)	Quality Factor	% Error in Resonant Frequency	% Error in Quality Factor	% Error (2^{15} time steps)	% Error (2^{12} time steps)
9.2723	999.5	0.0086	0.3	0.17	0.15
14.662	1580.3	0.034	1.8	0.027	0.99
16.145	1740.2	0.08	0.2	0.13	0.59
17.426	1878.3	0.02	0.17	0.052	0.86
20.800	2241.9	0.45	1.49	0.413	0.63
23.699	2560.5	0.22	0.29	0.39	0.29
25.501	2748.6	0.28	0.77	0.32	0.80

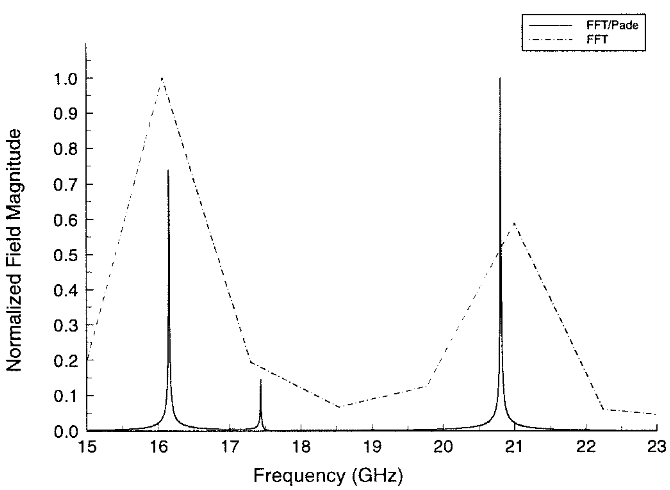

Fig. 3. Normalized frequency response of rectangular cavity for 1024 time iterations.

the CPU time requirement considerably as compared to the conventional FFT approach. For instance, the representative example shows that a reduction of eight orders-of-magnitude in CPU time can be achieved by using this new combinational technique relative to the ordinary FFT scheme. This method has also been tested for the canonical problem of an ideal lossless cavity with an infinite Q but the results are not presented here due to space limitations. The level of accuracy for the ideal case is nearly the same as that for the example presented herein. Finally, this scheme is not very sensitive to the choice of input parameters, and is feature makes it suitable as a module for a general-purpose FDTD simulation package.

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