Computation of Resonant Frequencies and Quality Factors of Cavities by FDTD Technique and Padé Approximation

Wei-Hua Guo, Wei-Jun Li, and Yong-Zhen Huang

***Abstract*—The finite-difference time domain (FDTD) technique and the Padé approximation with Baker's algorithm are used to calculate the mode frequencies and quality factors of cavities. Comparing with the fast Fourier transformation/Padé method, we find that the Padé approximation and the Baker's algorithm can obtain exact resonant frequencies and quality factors based on a much shorter time record of the FDTD output.**

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

I. Introduction

The finite-difference time-domain (FDTD) technique [1] is a powerful tool to calculate the resonant frequencies and quality factors for complex cavity structures, however, it is very time consumption. To save the computation time of the FDTD process, the Prony's method [2], the generalized pencil-of-function method [3], and the fast Fourier transform (FFT)/Padé method [4], [5] have been applied. The former two methods, which represent the time signal of FDTD as the sum of exponents, have advantages over FFT in terms of the reduction of the computation time, but their accuracy is sensitive to the sampling condition [4]. In this letter, the Padé approximation and the Baker's algorithm are applied to calculate the resonant frequencies and quality factors for resonant cavities. We find that the new method can achieve accuracy results by using a much shorter FDTD output sequence than the FFT/Padé method, especially for a cavity with adjacent modes.

II. Theory

Assuming that $u(n\Delta t)$ is the time response of one of the electromagnetic field components obtained from the FDTD technique, we can calculate its discrete Fourier transform by

$$U(\infty, f) = \sum_{n=0}^{\infty} u(n\Delta t)\exp(-i2\pi f n\Delta t) \tag{1}$$

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The authors are with State Key Laboratory on Integrated Optoelectronics, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100 083, China (e-mail: yzhuang@red.semi.ac.cn).

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where Δt is the FDTD time step. Now we introduce the Padé approximation to calculate (1) by defining

$$F(z,f) = \sum_{n=0}^{\infty} C_n z^n \tag{2}$$

$$C_n = u(n\Delta t)\exp(-i2\pi f n\Delta t). \tag{3}$$

It is evident that $F(1,f)$ is just $U(\infty,f)$. The diagonal Padé approximant $[N/2, N/2](z)$ of $F(z,f)$ at a certain frequency can be constructed from $C_n, n = 0, 1, \ldots, N$ (N is assumed to be an even number). It is known that the Padé approximation can be used to approximate the series from which it is generated [6], so we use $[N/2, N/2](1)$ as an approximation of $F(1,f)$, i.e., $U(\infty,f)$. The Padé approximant $[N,M](z)$ is defined as [6]

$$[N,M](z) = \frac{\sum_{n=0}^{M} a_n z^n}{\sum_{n=0}^{N} b_n z^n}. \tag{4}$$

The Baker's algorithm for calculating the nominator and the denominator of (4) is defined as [6]

$$[j, N-j](z) = \frac{\eta_{2j}(z)}{\theta_{2j}(z)} \tag{5}$$

$$[j, N-j-1](z) = \frac{\eta_{2j+1}(z)}{\theta_{2j+1}(z)} \tag{6}$$

with the following recursion relations:

$$\frac{\eta_{2j}(z)}{\theta_{2j}(z)} = \frac{\bar{\eta}_{2j-1}\eta_{2j-2}(z) - z\bar{\eta}_{2j-2}\eta_{2j-1}(z)}{\bar{\eta}_{2j-1}\theta_{2j-2}(z) - z\bar{\eta}_{2j-2}\theta_{2j-1}(z)} \tag{7}$$

$$\frac{\eta_{2j+1}(z)}{\theta_{2j+1}(z)} = \frac{\bar{\eta}_{2j}\eta_{2j-1}(z) - \bar{\eta}_{2j-1}\eta_{2j}(z)}{\bar{\eta}_{2j}\theta_{2j-1}(z) - \bar{\eta}_{2j-1}\theta_{2j}(z)} \tag{8}$$

where $\bar{\eta}_j$ is the coefficient of the highest power of z in $\eta_j(z)$ (i.e., $z^{N-[(j+1)/2]}$). The starting values of the recursion relations are given by

$$\eta_0(z) = \sum_{n=0}^{N} c_n z^n, \quad \theta_0(z) = 1.0$$

$$\eta_1(z) = \sum_{n=0}^{N-1} c_n z^n, \quad \theta_1(z) = 1.0. \tag{9}$$

Because $1/\Delta t$ is much larger than our interested frequency, the original FDTD output can be filtered and decimated to result a short input sequence for saving the computing time of the Padé approximation.

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TABLE I
RESONANT FREQUENCIES AND QUALITY FACTORS OF THE DOMINANT MODES

Analytical		Padé approximation (2^{11} time steps)			
Resonant Frequency (GHz)	Quality Factor	Resonant Frequency (GHz)	Quality Factor	% Error in Resonant Frequency	% Error in Quality Factor
9.3015	1002.5	9.3009	1002.3	0.006	0.02
14.707	1585.1	14.701	1584.4	0.04	0.04
17.113	1844.3	17.106	1842.5	0.04	0.10
18.603	2005.0	18.597	2004.3	0.03	0.03
20.799	2241.6	20.773	2240.2	0.12	0.06
23.714	2555.9	23.696	2554.0	0.07	0.07
25.277	2724.3	25.263	2720.0	0.05	0.16

III. NUMERICAL RESULTS

A rectangular cavity with nonloss walls, filled with a slightly lossy medium with the conductivity $\sigma = 5.1617 \times 10^{-4}$ s/m, is taken as an example. The side lengths of the cavity are taken to be 2.280, 1.044, and 2.280 cm, respectively. In the FDTD simulation, the spatial discretizations are chosen as 0.057, 0.058, and 0.057 cm in the three directions, respectively, and the time step is taken to be $\Delta t = 1.103 \times 10^{-12}$ s. We record the time response of one of the field components as the FDTD output, and then filter and decimate it at the rate of 1/8 to obtain an input sequence. The mode frequencies and quality factors are obtained from the peak frequencies and the ratio of the peak frequencies to the corresponding width of the intensity spectrum, which is obtained by the Padé approximation with the Baker's algorithm. In Table I, we present the numerical results of the resonant frequencies and the quality factors for dominant modes based on a 2^{11}-item FDTD output. We find that the exact results can be obtained from a half of the length of the FDTD output required in the FFT/Padé method [4].

To examine the effects of the degree of the diagonal Padé approximation, i.e., $N/2$, and the decimation rate on the accuracy of the results, we choose TE_{203} mode with the frequency of 23.714 GHz as an example. For the decimation rate of 1/4, 1/8, and 1/16, we find that the degree of $N/2 = 130$, 70, and 50 are required to obtain stable results, respectively. The corresponding lengths of the FDTD output are 1041, 1121, and 1601. In Fig. 1, we plot the percentage error of the quality factor as the functions of the length of the FDTD output. For the FFT/Padé method, 13 data samples are used in the interpolation process as in [4], and the decimation rate is taken to be 1/8 for the new method. The quality factor with percent error less than 0.1% can be obtained from a 1500-item FDTD output in the new method. However, the FFT/Padé method requires a 3500-item FDTD output to produce a quality factor with the same accuracy.

Finally, we consider a rectangular cavity with the side length of 2.280, 1.044, and 2.2804 cm, and the electrical conductivity of 5.1617×10^{-6} s/m. In the new cavity, two originally degenerative modes of TE_{103} and TE_{301} split with the frequency difference of 0.014%. The record of one electric field component in a fixed point versus the computation time is plotted in Fig. 2, the solid line is the FDTD output, and the circles are the input sequence after filtering and decimating the output with the rate of 1/8. In the calculation of Padé approximation, we usually discard the initial data during the excitation period. The first ten data is dropped in this case. Fig. 3 shows the spectral distributions of the field amplitude obtained by the new method and the FFT/Padé method. With a 5201-item FDTD output, we can get the quality factors for the two adjacent modes with the percentage error less than 0.06% under the new method. To obtain the same accuracy value of the quality factor, we require a 2^{15}-item FDTD output in the FFT/Padé method, which is about six times of that required in the new method. And we have about 20% errors in the quality factors obtained from the FFT/Padé method based on a 2^{14}-item FDTD output. In the FFT/Padé method, the FFT is carried out for the FDTD output, and then

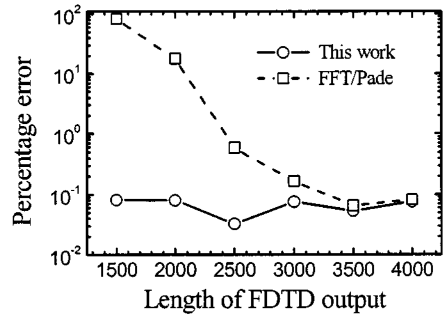

Fig. 1. Percentage errors of the quality factor for the TM_{203} mode obtained by the new method and the FFT/Padé method, versus the length of the FDTD time records.

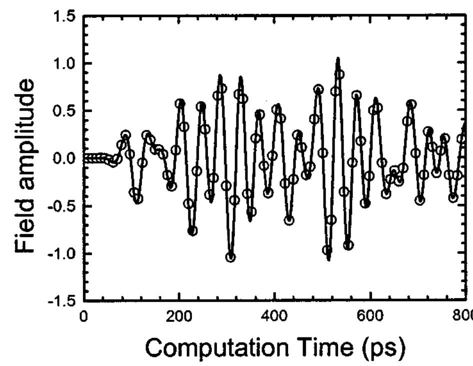

Fig. 2. FDTD output of one electric field component in a fixed point versus the computation time. The solid line is the original output, and the circles are the input sequence after filtering and decimating the output at the rate of 1/8.

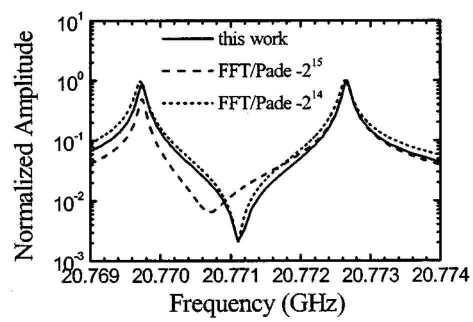

Fig. 3. Spectral distributions for the splitted TE_{103} and TE_{301} modes, obtained by the new method with a 5201-item FDTD output, and by the FFT/Padé method using 2^{14} and 2^{15}-item FDTD outputs, respectively.

the resolution of the spectral response of the FFT output is improved by the Padé approximation. In the new method, the Padé approximation with Baker's algorithm is directly applied to the FDTD output to yield the spectrum distribution at each frequency. Some frequency information in the FDTD output may be lost after FFT process, so FFT/Padé method need a longer FDTD output than the new method.

IV. Conclusion

We applied the FDTD technique and the Padé approximation to calculate the mode frequencies and quality factors of cavities. The Baker's algorithm, which directly calculates the nominator and denominator of the Padé approximation by recursion relations, are used to calculate the amplitude spectrum of the electromagnetic fields. Comparing with the FFT/Padé method, we find that the new method can reduce the computation time of the FDTD process more than the FFT/Padé method, especially for the cavity with adjacent modes.

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