TABLE II
EFFECTIVE DIELECTRIC CONSTANT FROM THIS PAPER AND [6] USING FIVE BASIS FUNCTIONS FOR J_z AND FOUR FOR J_x ($\varepsilon_r = 8$, $W/H = 1$, $\mu_r = 1$)

H/λ_0	This work	[6]
0.005	5.4678	5.4752
0.05	6.1275	6.1316
0.1	6.7580	6.7572
0.3	7.6614	7.6551
0.7	7.9139	7.9151
1.0	7.9529	7.9556

Here, I_0 and K_0 are modified Bessel functions of the first and second kind of order zero. This completes the evaluation of the asymptotic terms. Note that we are not particularly concerned with the Green's function G itself, but rather with the evaluation of the integrals, which naturally involve G, as they affect the solution.

IV. NUMERICAL RESULTS

SAT is used to determine the effective dielectric constant of the microstrip line of Fig. 1.

The effective dielectric constant of a microstrip line of aspect ratio $W/H = 1$ was determined for different values of the ratio H/λ_0. Table II summarizes the results obtained from five basis functions for J_z and four basis functions for J_x. The agreement between the results from this paper and those presented in [6] is excellent.

The numerical evaluation of the integrals with the proper asymptotic term subtracted and integrated in closed form was carried out using Gauss quadratures. All wavenumbers α, β are scaled in unit of the wavenumber in free space k_0. The upper limit of integration over the thus scaled variable α was determined as the maximum of $2\epsilon_r$ and $8\pi\lambda_0/H$. These two numbers are chosen to guarantee that all terms in the Green's dyadics have reached their asymptotic expressions, thereby leaving vanishing integrands for values of α larger than this upper limit.

The root of the determinant was located using the bisection method where the root is first bracketed starting from a value equal to the dielectric constant.

To reduce CPU times, the Fourier transforms of the basis functions are evaluated only once at the beginning of the program and stored in the computer's memory. Indeed, these are independent of β and keep the same values at each iteration in the search for the root of the determinant. Overall, 96 Gaussian points were used over the interval of integration, thereby requiring a memory space of the same size for each basis function. Within this implementation, the CPU time required to determine the effective dielectric constant is less than 100 ms per frequency point on an ULTRASPARC machine.

V. CONCLUSIONS

An SAT was introduced and applied to accelerate the analysis of dispersion properties of microstrip lines by the spectral-domain approach. Asymptotic forms of integrands are selectively extracted and evaluated in closed form without introducing additional numerical pathologies. Numerical results obtained from this approach agree well with those in the literature. A substantial reduction in CPU time is achieved by computing the Fourier transforms of the basis functions only once, in addition to subtracting the asymptotic parts of the integrands.

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On the Use of Linear-Prediction Techniques to Improve the Computational Efficiency of the FDTD Method for the Analysis of Resonant Structures

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***Abstract*—Linear-prediction (LP) techniques are used to accurately and efficiently compute the frequencies and damping factors of microwave resonant structures from their transient response, which was previously obtained by using the finite-difference time-domain (FDTD) method. The LP equations are formulated in terms of a total least squares (TLS) problem and are solved by using the singular-value decomposition (SVD) algorithm. This approach confers robustness to the LP method, improves the spectral resolution, and provides a simple criterion for selecting the order of the LP model. We illustrate these characteristics of the LP method by applying it to two types of problems: the determination of the propagation constants of waveguides loaded with lossy dielectrics, and the calculation of the resonant frequencies of cylindrical cavities loaded with dielectric ring resonators.**

***Index Terms*—FDTD, Maxwell solver, numerical methods.**

I. INTRODUCTION

The finite-difference time-domain (FDTD) method is a powerful numerical technique, which is currently used for the analysis of a

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wide variety of electromagnetic problems. For a given excitation waveform, this method directly provides the time-domain response of the structure under analysis. However, the spectral response is usually required for computer-aided design (CAD) purposes in microwave circuits. Traditionally, the frequency-domain results have been obtained by computing the fast Fourier transform (FFT) of the time-domain data. The main disadvantage of the FFT approach is the distortion of the spectral response that results from applying this approach to an FDTD response truncated in time. Therefore, the full FDTD response must be computed to obtain reliable results. Unfortunately, due to their high Q-factor, microwave circuits usually exhibit a very long transient response, which leads to time-consuming FDTD simulations. This limitation is particularly dramatic in resonant-type problems, where the accurate determination of the number of peaks in the spectral response (their locations and widths) is of capital importance.

To overcome the limitations of the FFT approach, a number of alternative spectral-analysis procedures have recently been proposed [1]–[7]. Roughly speaking, these methods are based on fitting the early FDTD response to a model. This allows the remaining part of the time-domain response to be computed by extrapolation, thus avoiding truncation problems. Additionally, the spectral response can be derived analytically by simply taking the z-transform of the model. The main problems with these methods are the difficulty involved in determining the order of the model, and their sensibility to noise in the data.

This paper discusses the application of the linear-prediction (LP) technique, which allows the parameters of interest to be extracted accurately and efficiently from the early FDTD response of resonant-type problems. These parameters are usually the resonant frequencies and the damping factors (or Q-factors) of the structure. The LP equations are formulated in the total least squares (TLS) sense and solved by using the singular-value decomposition (SVD) algorithm. This approach confers robustness to the LP technique and provides a simple and effective criterion for the selection of the order of the model. To illustrate the application of this technique, we have considered two types of resonant problems: the determination of phase and attenuation constants of waveguides loaded with lossy dielectrics, and the computation of resonant frequencies of cylindrical cavities loaded with dielectric ring resonators. For the first problem, the results are compared with those obtained using a commercial simulator based on the finite element (FE) method, while for the second one, comparisons are made with data available in the literature. For both cases, the agreement is found to be good.

II. Background of LP Techniques

A. The Underlying Signal Model

For a resonant structure, the FDTD transient response recorded at a fixed spatial point can be expressed as a superposition of complex exponentials

$$y(k\Delta t) \equiv y_k = x_k + n_k = \sum_{i=1}^{P} h_i \exp[(\delta_i + j2\pi f_i)k\Delta t] + n_k, \quad k = 0, \cdots, N-1 \quad (1)$$

where Δt is the FDTD time step, k is the time index, and y_k denotes the observed FDTD sequence of length N. The model parameters h_i, f_i, and δ_i represent the complex amplitude, frequency, and damping factor of the ith resonant mode, respectively. Since y_k is a real-valued sequence, the complex exponentials occur in conjugate pairs; hence, the order of the model P is twice the number of resonant modes. The sequence n_k accounts for the finite-precision errors of the FDTD simulation, the presence of nonexponential signals in y_k, and even exponential terms not included in x_k. The complex quantities $z_i = \exp(\delta_i + j2\pi f_i)\Delta t$ are the poles of the noiseless signal x_k.

B. The LP Technique

In this paper, an indirect method—the LP technique—is used to obtain the parameters of (1). This technique can be summarized in the following steps.

1) The true order P is not usually known beforehand, so an initial estimation of P, denoted by L, is chosen.
2) A TLS–LP problem is built up from the available time-domain data. For lossy structures, the backward approach is chosen, which leads to an $(N-L) \times (L+1)$ homogeneous system of linear equations. However, for lossless nonradiative structures, the forward–backward LP technique is used, resulting in an $2(N-L) \times (L+1)$ homogeneous system of linear equations [8].
3) The above TLS–LP problem is solved by using the SVD algorithm. The number of underlying exponentials (P) is estimated to be the number of the largest singular values of the data matrix. This is a simple and effective way to determine the order of the model, and is, in fact, a true noise-filtering process of the time-domain data [9].
4) The z-transform of the LP model is obtained. This allows the discrete-time Fourier transform of the time-domain data to be calculated without truncation problems by evaluating it on the unit circle of the z-plane. This procedure may be used in applications such as the calculation of S-parameters of microwave structures because, in these cases, only the shape of the spectral response is required. However, in resonant-type problems, the contribution of each single exponential term of (1) to the whole spectral response must be determined. To do this, the poles z_i of the z-transform of the LP model are computed.
5) Once the L poles z_i have been calculated, the P poles corresponding to the underlying exponentials must be separated from the others. For the backward formulation, the signal poles corresponding to the exponentials fall outside the unit circle in the z-plane, while the other poles remain inside the unit circle [10]. For the forward–backward formulation, the P poles closest to the unit circle are the signal poles [11].
6) Finally, the resonant frequencies and damping factor are computed directly from the signal poles.

III. Application of the LP Technique to FDTD Responses

A. Full-Wave Analysis of Guiding Structures

To obtain the dispersion characteristics of a uniform guiding structure, we adopt a transverse resonance approach [12], [13]. This approach consists of selecting a value of the phase constant β as an input parameter. The time-domain response to a given excitation waveform is computed and, finally, the resonant frequencies f_i and damping factors δ_i of the resonant modes are obtained by applying the techniques described in Section II. The pair of parameters (f_i, δ_i) corresponds to the ith propagating mode in such a way that at frequency f_i this mode has the value of β previously selected, and a value of the attenuation constant given by $\alpha_i = \delta_i / v_{gi}$, where v_{gi} is the group velocity. By changing the value of β and repeating this process, we can obtain the whole dispersion diagram.

To illustrate the application of the LP technique to compute the resonant frequencies and damping factors, we first consider the calculation of the dispersion characteristics of the TE_{n0} modes of

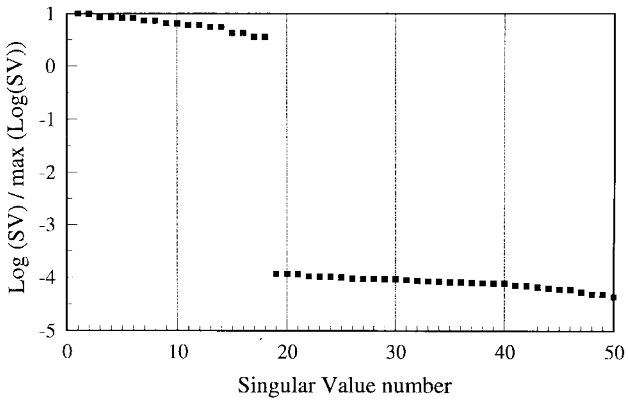

Fig. 1. Singular values for the TE_{n0} modes of WR-90 waveguide filled with a dielectric of $\epsilon_r = 1$ and $\sigma = 0.001$ S/m. FDTD mesh: ten unit cells. LP input parameters: $N = 100$, $D = 1$, and $L = 50$.

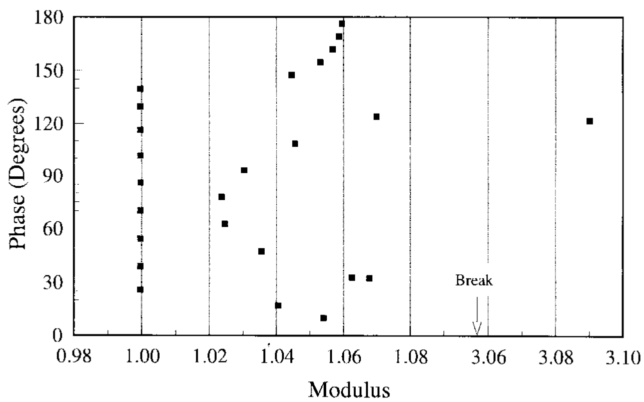

Fig. 2. Poles of the LP model for the same case as in Fig. 1.

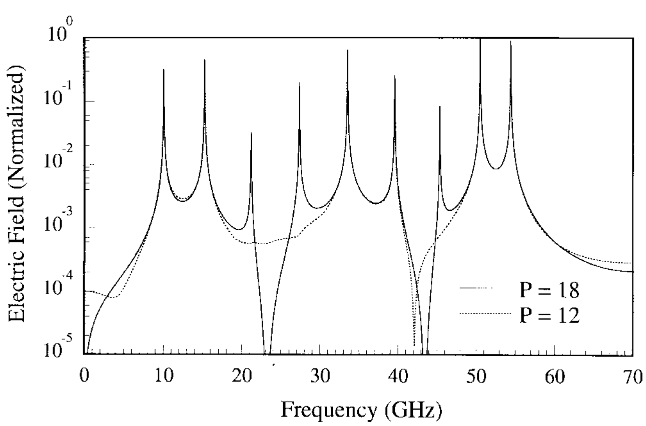

Fig. 3. Spectral response for the same structure as in Fig. 1.

a WR-90 waveguide completely filled with a lossy dielectric material of dielectric constant $\epsilon_r = 1$ and conductivity $\sigma = 0.001$ S/m. This structure is discretized using an FDTD mesh of only ten unit cells. Initial conditions are imposed at the grid point $x = 3\Delta x$, where Δx is the spatial step. The FDTD response for $\beta = 158.24$ rad/m (the exact value of β for the TE_{10} mode at 10 GHz) is recorded at $x = 7\Delta x$. In this case, as a consequence of the chosen spatial discretization and of the simplicity of the structure, we know beforehand that the number of resonant modes is nine and, hence, the order of the model is $P = 18$. To verify this value, we have carried out an SVD of the data matrix by using the first 100 samples of the FDTD response and a value for the initial order of $L = 50$. The singular values, computed by using the backward LP formulation, are shown in Fig. 1. They have been sorted in decreasing order. As expected, there are 18 dominant singular values, which determine the order of the model. A large gap is observed between the dominant singular values and all the others. Fig. 2 shows the poles of the LP model. They have been reflected with respect to the unit circle of the z-plane, so that the poles having modulus less than one correspond to the waveguide modes. For clarity, only half of the poles have been plotted, the remaining poles are their complex conjugates. Finally, the spectral response of the structure is plotted in Fig. 3 for the whole Nyquist range. There are two curves: the solid curve was obtained with $P = 18$ (the correct order), and the dashed curve with $P = 12$ (retaining the first 12 singular values). It can be seen that an underestimation of P produces a true filtering of the spectral response. We have observed that the highest singular values belong to the modes with the largest amplitudes; therefore, the filtered modes are those that have the smallest amplitudes. However, this filtering process affects all modes, in this case, mainly acting on their damping factors.

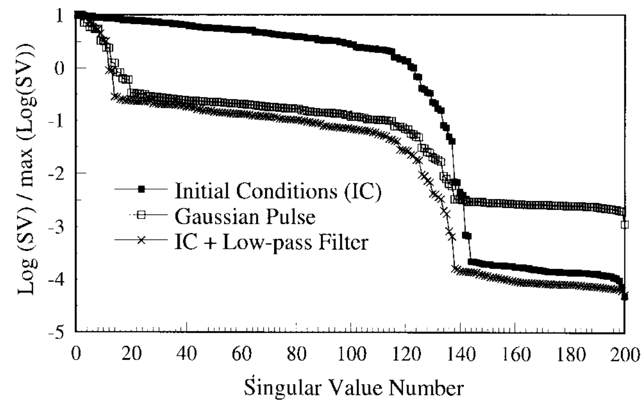

Fig. 4. Singular values for the TE_{nm} modes of a WR-90 waveguide filled with a dielectric of $\epsilon_r = 1$ and $\sigma = 0.001$ S/m. FDTD mesh: 10×10 unit cells. LP input parameters: $N = 400$, $D = 1$, $L = 200$. Three different cases are shown: using initial conditions, Gaussian pulse, and low-pass filtering of the FDTD response.

For more complex structures, the number of excited modes and, hence, the order of the model, is usually excessively large. For example, if we simply consider the same WR-90 waveguide of the previous example as a two-dimensional (2-D) problem and use a discretization of 10×10 cells, the expected number of TE_{nm} modes is 81. To overcome this problem, we propose two different alternatives: using a Gaussian pulse to excite the problem structure or applying a low-pass digital filter to the FDTD response. Both approaches allow us to greatly attenuate the higher order modes. These modes are not of interest because they are not resolved with enough accuracy by the FDTD mesh. Fig. 4 shows the singular values obtained for this example with an initial order of $L = 200$. When using initial conditions, a nonabrupt transition is observed between the dominant singular values and all the others. For nonabrupt transitions, it is better to overestimate P, say, $P = 142$ for this case. If the guide is excited with a Gaussian pulse, we observe an additional gap, which is due to the fact that the Gaussian excitation concentrates the energy on the modes with lower resonant frequencies. This allows us to consider as dominant modes those that correspond to the first gap, so we can take a model order of about $P = 20$. The same situation is found when the time-domain signal is low-pass filtered. The higher the attenuation of the filter, the larger the gap obtained in the magnitude of the singular values. For a larger gap, the accuracy obtained in the exponential model parameters is better. Both the pulse

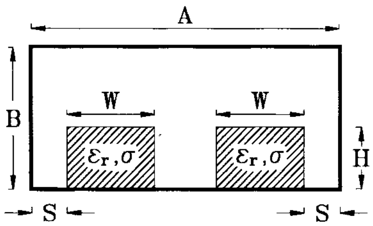

Fig. 5. WR-90 waveguide loaded with two H-plane dielectric slabs. $A = 22.86$ mm, $B = 10.16$ mm, $W = A/4$, $S = A/8$, $H = B/6$, $\epsilon_r = 12$, $\sigma = 0.1$ S/m.

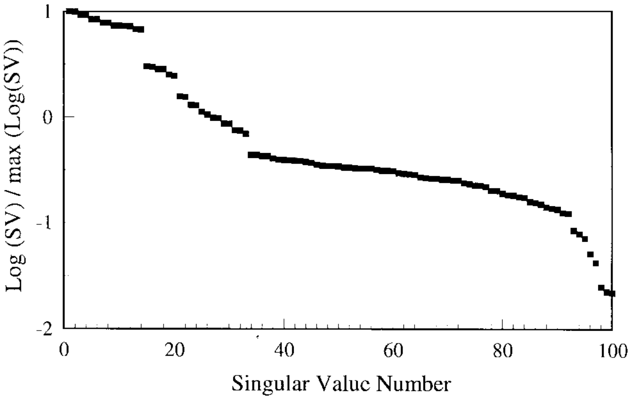

Fig. 6. Singular values for the structure shown in Fig. 5. FDTD mesh: 48 × 36 cells. Excitation: Gaussian pulse. LP input parameters: $N = 200$, $D = 10$, and $L = 100$.

excitation and filtering approach are techniques that effectively reduce the order of the model. Furthermore, these techniques allow lower values for L to be used, improving the efficiency of the LP method.

As an example of a structure of more practical interest, we have considered a WR-90 waveguide loaded with two H-plane dielectric slabs. This structure is depicted in Fig. 5. The simulations were carried out for $\beta = 183.17$ rad/m. The time-domain response was obtained by using a Gaussian excitation with a length of 400 FDTD samples. To perform the spectral analysis of the FDTD response, we consider a window of 2000 samples (from the 500th to the 2500th FDTD iteration). The time samples recorded while the excitation was switched on are not considered. Since FDTD usually gives oversampled responses, the data contained in the window are decimated with a decimation factor $D = 10$. In other words, only one in every ten samples is retained and, as a consequence, the number of samples is reduced to $N = 200$. Fig. 6 shows the singular values obtained with $L = 100$. From this figure, we estimate a model order of $P = 40$. The spectral response obtained for this case is plotted in Fig. 7. Table I shows the results obtained for the frequencies, damping factors, and attenuation constants of the first two modes of this structure. We have considered four different discretizations given by $8l \times 6l$ where l is a parameter that takes values 3, 4, 5, and 6, as shown in Table I. The curve

$$\xi(l) = A + \frac{B}{l} + \frac{C}{l^2} \tag{2}$$

has been used to model the convergence behavior of the results as a function of l, where ξ is the parameter of interest (frequency or attenuation factor) and A, B, and C are the constants to be determined. The extrapolated values for $l = \infty$ are also shown in Table I. These values are in excellent agreement with those obtained using a commercial simulator based on the FE method.[1]

[1] *High-Frequency Structure Simulator,* Release 3.0, Hewlett-Packard, Santa Rosa, CA.

TABLE I
COMPARISON OF RESULTS FOR THE WAVEGUIDE SHOWN IN FIG. 5 OBTAINED BY USING THE FDTD METHOD WITH SEVERAL SPATIAL DISCRETIZATIONS GIVEN BY $8l \times 6l$, AND BY USING THE HIGH-FREQUENCY STRUCTURE SIMULATOR (HFSS)

Mesh	1st mode			2nd mode		
l	f (GHz)	δ (ns^{-1})	α (Np/m)	f (GHz)	δ (ns^{-1})	α (Np/m)
3	9.959	0.0397	0.20	13.091	0.122	1.69
4	9.976	0.0436	0.22	13.140	0.131	1.82
5	9.984	0.0461	0.23	13.163	0.138	1.91
6	9.988	0.0478	0.24	13.177	0.142	1.97
∞	10.003	0.0576	0.29	13.214	0.167	2.32
HFSS	10.000	–	0.29	13.210	–	2.29

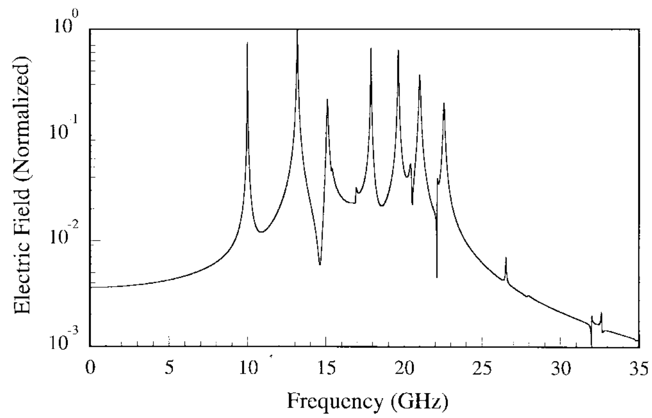

Fig. 7. Spectral response for the waveguide of Fig. 5 for $\beta = 183.17$ rad/m.

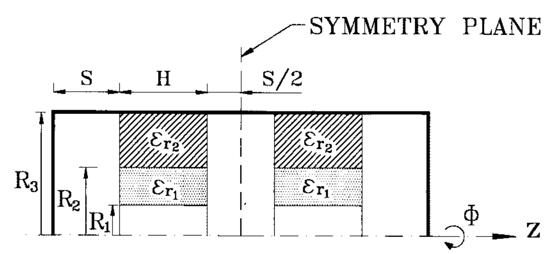

Fig. 8. Cylindrical cavity loaded with two dielectric ring resonators. $\epsilon_{r1} = 1.031$, $\epsilon_{r2} = 24.3$, $R_2 = 2.455$ mm, $R_1 = 0.3R_2$, $R_3 = 2.39R_2$, $H = 3.61$ mm, $S = 2H$.

B. Characterization of Dielectric Resonators

The second resonant-type problem addressed in this paper is the characterization of cavities loaded with dielectric resonators. In particular, we consider the computation of the resonant frequencies of the TE_{01} modes of a cylindrical cavity loaded with two ring dielectric resonators, as shown in Fig. 8. An accurate determination of the resonant frequencies is important in order for the mutual coupling factor of the resonators to be obtained. This can be done by taking advantage of the symmetry of the structure. First, the problem is solved with a perfect electric wall in the symmetry plane; then, it is solved again with a perfect magnetic wall. The solutions obtained in

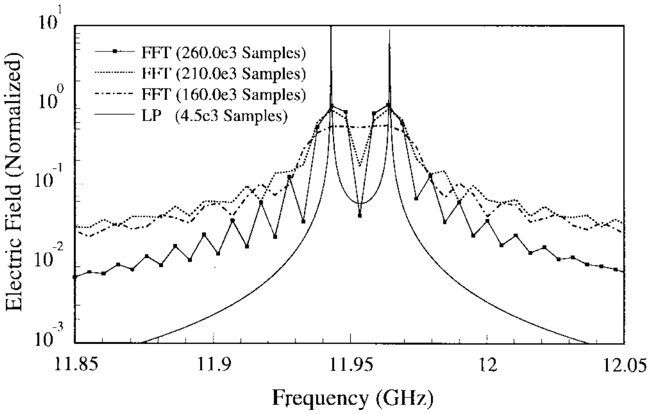

Fig. 9. Spectral response for the TE_{01} modes of the structure shown in Fig. 8. Results were calculated using the FFT method with 160 000, 190 000, and 210 000 FDTD samples, and using the LP method with 4500 FDTD samples.

each case are labeled as TE_{01e} and TE_{01h} modes, respectively. The coupling factor is calculated simply as

$$k \simeq 2\frac{f_{01e} - f_{01h}}{f_{01e} + f_{01h}}. \tag{3}$$

However, to show the resolution improvements of the LP technique with respect to the FFT method, we have analyzed this structure without considering symmetries (the resonant frequency of the two modes are obtained in the same simulation). We have used an FDTD mesh of 48 × 80 cells. The size of the unit cell is $\Delta r = 0.122\,75$ mm and $\Delta z = 0.361$ mm. The structure has been excited with a Gaussian pulse with a length of 800 FDTD samples. Since we are analyzing a lossless structure, the resonant frequencies have been computed by using the forward–backward LP formulation. We have considered a window with data from the 1000–4500th FDTD iteration. The parameters used are $D = 25$ and $L = 70$. When the FDTD response is highly oversampled (as in this case), the use of high decimation factors is a way of improving the resolution of the LP method [14]. Ideally, the frequency band of interest should be expanded in the whole Nyquist range. The spectral response obtained for the TE_{01e} and TE_{01h} modes is shown in Fig. 9. This figure also shows the results obtained by using the FFT method for different numbers of FDTD iterations. It can be seen that with the FFT method at least 160 000 FDTD samples are required to discriminate the two peaks. For the curves computed by the FFT approach, we have applied zero padding to 512 000 data samples. Table II compares the results for the resonant frequencies and the coupling factor computed by using the FDTD method in two different situations: analyzing the whole structure in one simulation, and taking into account the symmetry wall to perform the analysis in two different simulations, thus avoiding problems of spectral resolution. These results are also compared with those obtained by using the mode-matching (MM) method [15], showing good agreement. Note that we are using a uniform FDTD mesh and, hence, the radius of the cavity has been approximated by $R_3 \simeq 48\Delta r = 5.892$ mm, which means there is an error of 0.46% in this dimension.

TABLE II
COMPARISON OF THE RESULTS CALCULATED FOR THE STRUCTURE SHOWN IN FIG. 8 USING THE FDTD METHOD AND THE MM METHOD. FOR THE FDTD METHOD, THE RESULTS HAVE BEEN OBTAINED IN ONE SIMULATION (*), AND IN TWO SIMULATIONS, TAKING INTO ACCOUNT THE SYMMETRY WALL (**)

	FDTD*	FDTD**	MM [16]
f_{01e} (GHz)	11.9646	11.9646	11.9684
f_{01h} (GHz)	11.9431	11.9429	11.9476
k	$1.80\ 10^{-3}$	$1.82\ 10^{-3}$	$1.74\ 10^{-3}$
$f_0 = \sqrt{f_{01e}\, f_{01h}}$	11.9538	11.9537	11.9580

IV. CONCLUSION

This paper has dealt with the way LP techniques can be applied to obtain the frequencies and damping factors from the FDTD response of resonant structures. The formulation adopted is based on expressing the LP problem in the TLS sense and solving the resulting set of homogeneous linear equations by means of the SVD algorithm. This approach provides an effective criterion for determining the order of the model. For lossy structures, the backward LP technique is used. This provides a simple way of separating the poles that correspond to the resonant modes from the rest. For lossless structures, the forward–backward LP method is applied. It has been shown that in the case where the order of the model is too high, it can be reduced by using a pulse waveform to excite the structure in the FDTD simulation or by low-pass filtering the time-domain response. These techniques for reducing the model order improve the efficiency of the method. It has also been shown that in cases where two resonances are very close to each other, the LP method is still capable of computing them with good accuracy and from relatively short FDTD responses. By contrast, when the same situation is handled using the FFT method, we need sequences that are at least some 35 times longer.

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