The Finite-Difference–Time-Domain Method and its Application to Eigenvalue Problems

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Abstract —**This paper describes the application of the finite-difference method in the time domain to the solution of three-dimensional (3-D) eigenvalue problems. Maxwell's equations are discretized in space and time, and steady-state solutions are then obtained via Fourier transform. While achieving the same accuracy and versatility as the TLM method, the finite-difference–time-domain (FD–TD) method requires less than half the CPU time and memory under identical simulation conditions. Other advantages over the TLM method include the absence of dielectric boundary errors in the treatment of 3-D inhomogeneous planar structures, such as microstrip. Some numerical results, including dispersion curves of a microstrip on anisotropic substrate, are presented.**

I. Introduction

The TLM METHOD has been successfully applied to various microwave circuit problems for more than ten years. The special advantages of the TLM technique over other numerical methods are well illustrated by Johns and Beurle [1] in their original paper on the method. Since then, several improvements have been made to this technique by various authors in order to enhance the accuracy of the solution and economize CPU time and memory space [2]–[5]. Mariki [7] has extended the TLM method to analyze anisotropic media, and Saguet and Pic [4] as well as Al-Mukhtar and Sitch [5] have employed a graded mesh to make the algorithm faster and more efficient.

Although the graded mesh algorithm reduces memory space requirements, it demands far more iterations than the original method for equal frequency resolution [5]. This is especially obvious in the case of three-dimensional (3-D) simulations where the grade ratio N requires an additional N^2-1 iterations. These requirements of large computer resources may critically limit the applicability of the TLM technique.

Thus, Saguet [16] has proposed a simplified node which reduces the number of variables to be processed and stored at each node by one third. However, this modification increases the velocity error. A further reduction in computational expenditure has been proposed by the authors [8]; instead of the original vector solution, we obtain a scalar potential solution using a scalar 3-D network. However, the scalar approach is limited to problems which lead to uncoupled modal solutions, i.e., TE and TM or LSE and LSM fields.

The major reason for the large CPU memory demand of this technique resides in the basic 3-D TLM concept. In order to represent each electromagnetic component, each 3-D unit cell requires 26 real memory spaces, 12 for pulse storage and 14 for additional network parameters. Therefore, each operation on each node involves a large number of variables, requiring considerable computer CPU space and time. Furthermore, experience has shown that the number of iterations increases with the complexity of the structure under study. For example, the accurate analysis of a finline requires easily over 1000 iterations. Given these massive requirements, we have searched for an alternative numerical technique that possesses the advantages of the TLM approach but needs fewer computer resources. As a result, a new algorithm is proposed based on both the finite-difference–time-domain (FD–TD) and TLM methods.

The FD–TD method was first formulated by Yee [6], and has been applied extensively to scattering and coupling problems with open boundaries [9]–[15], i.e., to the solution of deterministic problems. We noted the similarity between this method and the TLM method, which has been widely used in the numerical solution of the electromagnetic eigenvalue problems in the time domain. Since the TLM method is based on the computation of the impulse response of a large mesh of transmission lines, much unwanted information is usually generated.

We have therefore developed a novel procedure which increases the numerical efficiency of the time-domain approach without sacrificing its advantages. The method differs from the classical FD–TD method in the assignment of initial field values and the application of the Fourier transform to the time-domain solution. In the following, we will describe this method and its application to some typical microwave problems.

II. Yee's Algorithm

Maxwell's equations have been expressed in finite-difference form by Yee [6] to solve two-dimensional (2-D) wave scattering problems. Subsequently, 3-D scattering problems have been solved by Taflove and other workers

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[9]–[15]. We will adopt Yee's original algorithm for the three-dimensional Maxwell's equations. Also, we will extend the concept further to include anisotropic media.

In a rectangular coordinate system, the source-free Maxwell's equations can be written as first-order hyperbolic equations

$$d\bar{E}/dt = |A_x|\, d\bar{H}/dx + |A_y|\, d\bar{H}/dy + |A_z|\, d\bar{H}/dz$$
$$d\bar{H}/dt = |B_x|\, d\bar{E}/dx + |B_y|\, d\bar{E}/dy + |B_z|\, d\bar{E}/dz \qquad (1)$$

where $\bar{E} = (E_x, E_y, E_z)^t$, $\bar{H} = (H_x, H_y, H_z)^t$, and

$$|A_x| = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\epsilon_{yy}^{-1} \\ 0 & \epsilon_{zz}^{-1} & 0 \end{bmatrix}, |A_y| = \begin{bmatrix} 0 & 0 & \epsilon_{xx}^{-1} \\ 0 & 0 & 0 \\ -\epsilon_{zz}^{-1} & 0 & 0 \end{bmatrix}$$

$$|A_z| = \begin{bmatrix} 0 & -\epsilon_{xx}^{-1} & 0 \\ \epsilon_{yy}^{-1} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Here, ϵ_{xx}, ϵ_{yy}, and ϵ_{zz} are the diagonal elements of the permittivity tensor. All B_x, B_y, and B_z are expressed by replacing ϵ_{xx}, ϵ_{yy}, and ϵ_{zz} by $-\mu_{xx}$, $-\mu_{yy}$, and $-\mu_{zz}$ components, which are the diagonal elements of the permeability tensor. Then each of these scalar equations can be expressed in finite-difference form. Following Yee's nomenclature, any function of space and time is discretized

$$F^n(i, j, k) = F(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$$

where $\Delta x = \Delta y = \Delta z = \Delta l$ is the space increment and Δt is the time increment. By positioning the components of $\bar{E}$ and $\bar{H}$ on the mesh as depicted in Fig. 1 and evaluating $\bar{E}$ and $\bar{H}$ at alternate half time steps, we obtain the components of Maxwell's equations.

$$\begin{aligned} H_x^{n+1/2}&(i, j+1/2, k+1/2) \\ &= H_x^{n-1/2}(i, j+1/2, k+1/2) \\ &\quad + s/\mu_{xx}(i, j+1/2, k+1/2)\big[E_y^n(i, j+1/2, k+1) \\ &\quad - E_y^n(i, j+1/2, k) + E_z^n(i, j, k+1/2) \\ &\quad - E_z^n(i, j+1, k+1/2)\big] \end{aligned} \qquad (2a)$$

$$\begin{aligned} H_y^{n+1/2}&(i+1/2, j, k+1/2) \\ &= H_y^{n-1/2}(i+1/2, j, k+1/2) \\ &\quad + s/\mu_{yy}(i+1/2, j, k+1/2)\big[E_z^n(i+1, j, k+1/2) \\ &\quad - E_z^n(i, j, k+1/2) + E_x^n(i+1/2, j, k) \\ &\quad - E_x^n(i+1/2, j, k+1)\big] \end{aligned} \qquad (2b)$$

$$\begin{aligned} H_z^{n+1/2}&(i+1/2, j+1/2, k) \\ &= H_z^{n-1/2}(i+1/2, j+1/2, k) \\ &\quad + s/\mu_{zz}(i+1/2, j+1/2, k)\big[E_x^n(i+1/2, j+1, k) \\ &\quad - E_x^n(i+1/2, j, k) + E_y^n(i, j+1/2, k) \\ &\quad - E_y^n(i+1, j+1/2, k)\big] \end{aligned} \qquad (2c)$$

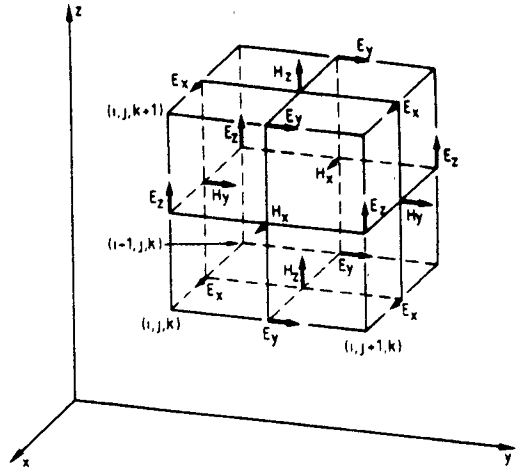

Fig. 1. The position of the field components in Yee's mesh.

$$\begin{aligned} E_x^{n+1}&(i+1/2, j, k) \\ &= E_x^n(i+1/2, j, k) + s/\epsilon_{xx}(i+1/2, j, k) \\ &\quad \cdot\big[H_z^{n+1/2}(i+1/2, j+1/2, k) \\ &\quad - H_z^{n+1/2}(i+1/2, j-1/2, k) \\ &\quad + H_y^{n+1/2}(i+1/2, j, k-1/2) \\ &\quad - H_y^{n+1/2}(i+1/2, j, k+1/2)\big] \end{aligned} \qquad (2d)$$

$$\begin{aligned} E_y^{n+1}&(i, j+1/2, k) \\ &= E_y^n(i, j+1/2, k) + s/\epsilon_{yy}(i, j+1/2, k) \\ &\quad \cdot\big[H^{n+1/2}(i, j+1/2, k+1/2) \\ &\quad - H_x^{n+1/2n}(i, j+1/2, k-1/2) \\ &\quad + H_z^{n+1/2}(i-1/2, j+1/2, k) \\ &\quad - H_z^{n+1/2}(i+1/2, j+1/2, k)\big] \end{aligned} \qquad (2e)$$

$$\begin{aligned} E_z^{n+1}&(i, j, k+1/2) \\ &= E_z^n(i, j, k+1/2) + s/\epsilon_{zz}(i, j, k+1/2) \\ &\quad \cdot\big[H_y^{n+1/2}(i+1/2, j, k+1/2) \\ &\quad - H_y^{n+1/2}(i-1/2, j, k+1/2) \\ &\quad + H_x^{n+1/2}(i, j-1/2, k+1/2) \\ &\quad - H_x^{n+1/2}(i, j+1/2, k+1/2)\big] \end{aligned} \qquad (2f)$$

where the stability factor $s = c\Delta t/\Delta l$, and c is the velocity of light. In these expressions, E and H are normalized such that the characteristic impedance of space is unity. The condition for stability of (1) in free space is [10]

$$s \leqslant 1/\sqrt{3}. \qquad (3)$$

III. Boundary Conditions

So far, a space–time mesh has been introduced and Maxwell's equations have been replaced by a system of finite-difference equations. Difficulties arise when the domain in which the field must be computed is unbounded. Since no computer can store an unlimited amount of data, a special technique must be used to limit the domain in which the numerical computation is made, by introducing so-called absorbing or soft boundary conditions. These conditions have been described by Taylor *et al.* [9], who use a simple extrapolation method, and by Taflove and Brodwin [10], who simulate the outgoing waves and use an averaging process in an attempt to account for all possible angles of propagation of the outgoing waves. Kunz and Lee [12] use the radiation condition at a large distance from the center of the scatterer to obtain an absorbing boundary condition. Mur [13] employs a second-order radiation condition to improve the accuracy of the results. Although these schemes have been used in scattering problems in the past, no ideal reflection-free boundary condition has been proposed so far.

However, in the formulation of eigenvalue problems, only "hard boundaries"—usually represented by conducting walls—occur. At these boundaries, the tangential electric and the normal magnetic field components are maintained at zero. For example, on a perfectly conducting wall in the plane $i=1$ (see Fig. 1)

$$\text{for all } n \begin{cases} E_y^n(1, j+1/2, k) = 0 \\ E_z^n(1, j, k+1/2) = 0 \\ H_x^n(1, j+1/2, k+1/2) = 0 \end{cases}$$

(the third condition is implicit in the previous two, but its implementation reduces numerical errors).

IV. Initial Values

In most scattering problems, an impulsive or sinusoidal plane wave is injected at the beginning of the computation. However, in eigenvalue problems, the direction of the propagation vector is usually not known and depends on the space coordinates and on the eigenvalue that is to be found. In these cases, the logical choice is an isotropic pulse that propagates in the radial direction. The spatial pulse envelope should be wide enough with respect to the mesh size not to accumulate numerical errors due to overshoot and ringing as it propagates through the space lattice.

A better way to start the computation is to estimate the field distribution of the desired mode in the structure first and then choose the initial value accordingly. The experienced researcher usually has a good idea of the approximate modal field distributions in a structure and is therefore able to make an educated guess of the steady-state field pattern for a particular eigenmode. This procedure is equivalent to the excitation of a TLM mesh with a weighted impulse distribution, and is somewhat similar to the way in which one chooses appropriate basis functions in the spectral-domain approach.

V. Outline of the Numerical Procedure

The application of the FD–TD method will be discussed using a rectangular resonator as an example. A continuous medium is replaced with a 3-D uniform mesh. To solve the system of equations (2) in this mesh, initial values must be assigned first as described in the previous section. For a rectangular-type resonator, a simple sinusoidal function is an appropriate choice for the dominant mode eigenvalue. As n increases, the discrete time functions for $\bar{E}$ and $\bar{H}$ fields evolve towards the steady state which is characteristic of the desired mode in the geometry. In this way, the evolution of all six field components is obtained simultaneously at discrete time points $n\Delta t$. The final steady-state field distribution may be calculated by taking the time average of the time-domain solution at each mesh point. Thus, the steady-state solution is given by

$$F(i_0, j_0, k_0) = \sum_n |F^n(i_0, j_0, k_0)|/N. \tag{4}$$

This simple procedure to obtain the final field distribution is another advantage over the TLM method, which requires two simulations for finding the fields of a given mode.

In eigenvalue problems, the steady-state solution is a time-harmonic function, from which the eigenvalues can

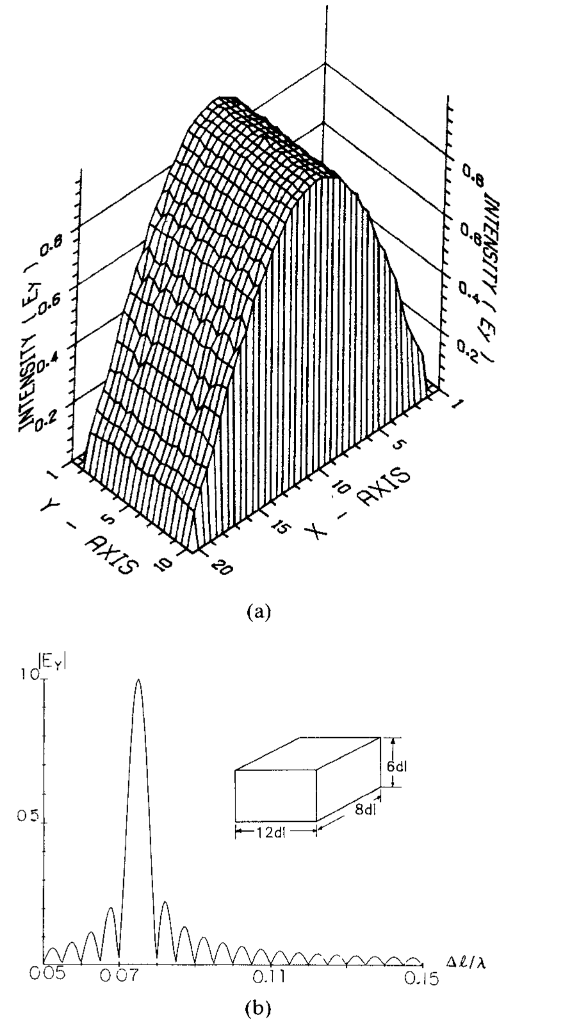

Fig. 2. (a) Field distribution of an empty rectangular resonator obtained with the FD–TD method. (b) Output spectrum obtained with both the FD–TD and TLM methods under identical conditions

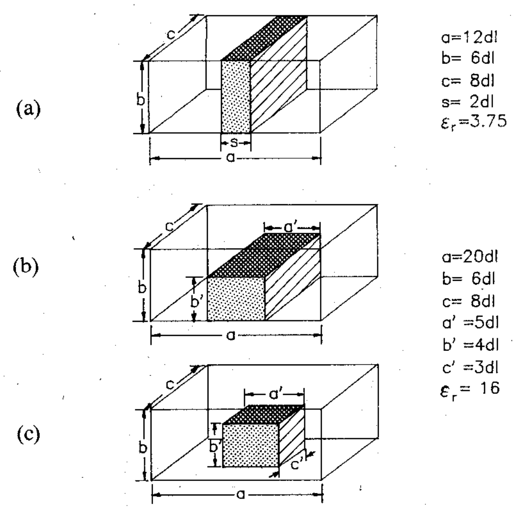

Fig. 3. Three-dimensional inhomogeneous resonators analyzed in this study.

TABLE I
COMPARISON OF RESULTS FOR THE NORMALIZED RESONANT FREQUENCIES $\Delta l/\lambda$ OBTAINED WITH THE TLM AND FD–TD METHODS UNDER IDENTICAL SIMULATION CONDITIONS FOR THE GEOMETRIES IN FIG. 3

Fig.3	Mode	s/a	TRM	TLM (CPU time)	FD–TD (CPU time)
a)	LSE	1/6	0.05220	0.0516 (144)	0.0517 (51)
		1/3	0.0445	0.0440 (145)	0.0442 (51)
b)	Hybrid			0.0278 (357)	0.0278 (117)
c)	Hybrid			0.0405 (357)	0.0405 (117)

be extracted by discrete Fourier transform, as in the TLM method

$$S(f) = \sum_n F^n(i_0, j_0, k_0) \exp(-j2\pi snf). \qquad (5)$$

Both the stability factor s and the number of iterations n strongly affect the spectral response.

In order to test this algorithm for validity, it has been applied to a simple rectangular cavity with sides $12\,\Delta l \times 6\,\Delta l \times 8\,\Delta l$. We have assumed a dominant TE_{101} mode in the initial value assignment. The time-domain solution is given in Fig. 2(a). Discontinuous field figures are due to the numerical error caused by the finite-difference form of (2). Fig. 2(b) compares the frequency responses obtained with the FD–TD and TLM methods under identical conditions. The responses are not distinguishable. Five hundred iterations have been used. The peak of the solution is located at $\Delta l/\lambda = 0.0750$ in both methods. The exact analytical solution is 0.07511. Even though a small number of meshes is used in this algorithm when compared with the scattering problems in [9]–[13], it is noted that the accuracy in the solution of the eigenvalue problems is better than that of the scattering problems by one order of magnitude.

VI. NUMERICAL RESULTS

We have applied this technique to most of the examples described in the TLM literature and obtained practically identical results. The method requires less than one-half of the CPU time spent by the equivalent TLM program under identical conditions, including the initial excitation distribution. Furthermore, while the TLM procedure requires 22 real memory stores per 3-D node in an isotropic dielectric, the FD–TD method requires only seven real memory stores per node. Fig. 3(a), (b), and (c) shows structures for which solutions have been computed with this method. The dominant resonant frequencies of these structures are given and compared with the TLM solution in Table I. The inhomogeneous rectangular cavity of Fig. 3 (b) and (c) illustrates the capability of this algorithm to solve hybrid field problems. The number of nodes chosen in each problem is the same as that employed in the TLM solution.

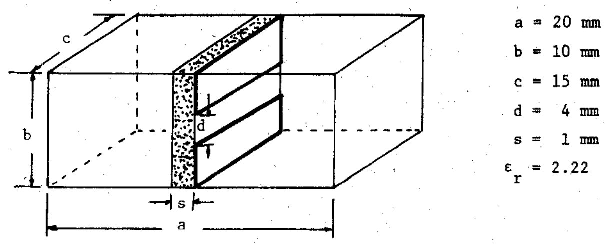

Fig. 4. Finline cavity.

TABLE II
RESONANT FREQUENCIES OF THE UNILATERAL FINLINE CAVITY IN FIG. 4, OBTAINED WITH VARIOUS METHODS

	Saguet [16]		This method	
	S.D.A.	Variable Mesh TLM	TDFD	T.L.M.
Resonant Frequency (GHz)	10.77	10.14	10.74	10.74
Number of Iterations		1000	600	600
CPU Time(s)			170	380

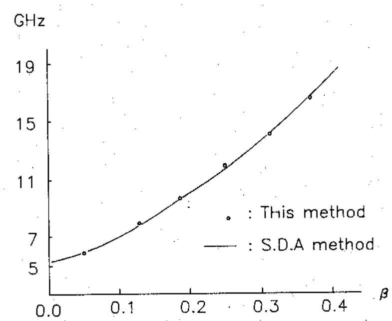

Fig. 5. Dispersion diagram of unilateral finline with the cross-sectional geometry given in Fig. 4.

Furthermore, we have computed the resonant frequency of a finline resonator (Fig. 4.) treated previously by Saguet [16]. Results are compared in Table II, which includes a value obtained with the spectral-domain method by Saguet. Fig. 5 shows the dispersion characteristics of a finline with the same cross section, as obtained with our method. Results calculated with our spectral-domain program are also shown in the same figure. In order to compare convergence of both time-domain methods, solutions obtained after every fifth iteration are drawn in Fig. 6. The results show virtually identical convergence.

To show the versatility of this method, the characteristics of a microstrip resonator on anisotropic substrate are

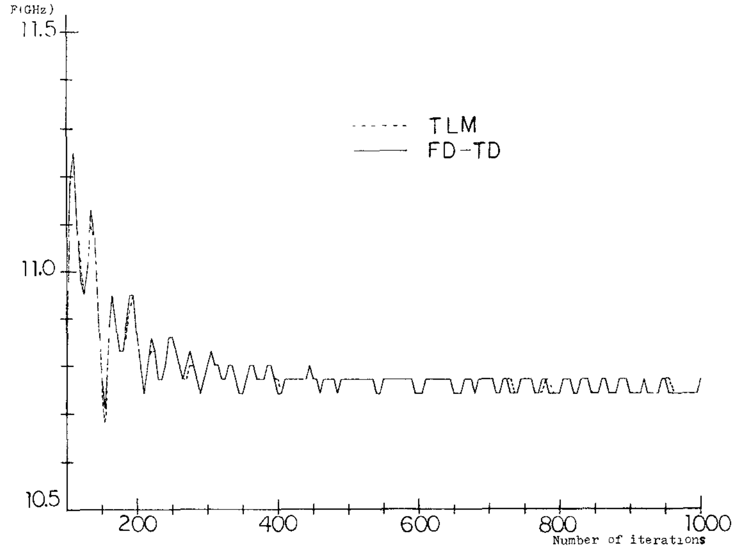

Fig. 6. Stability and convergence of the TLM and FD–TD methods as a function of the number of iterations. The solution of the finline problem in Fig. 4 is represented.

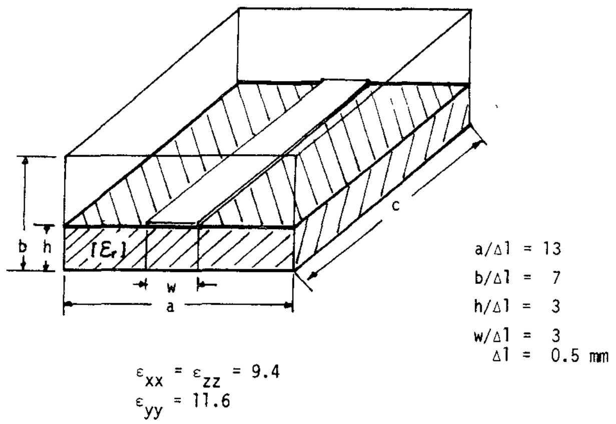

Fig. 7. Microstrip cavity on anisotropic substrate.

TABLE III
DOMINANT RESONANT FREQUENCIES OBTAINED BY BOTH THE TLM AND THE FD–TD METHODS

	h \ c/Δl	6	8	10	15	20
TLM (GHz)	3Δl	15.72	12.24	10.14	7.14	5.46
	4Δl	14.22	11.16	9.18	6.36	4.98
	Average	14.97	11.70	9.66	6.75	5.22
FD - TD (GHz)		14.64	11.52	9.54	6.78	5.28

computed in the last example, shown in Fig. 7. Several different resonant frequencies obtained by changing the length c are tabulated in Table III. It is well known [17] that the TLM simulation of 3-D inhomogeneous planar structures involves dielectric interface ambiguity. The best way to resolve this error is to employ two dielectric substrate thicknesses differing by one Δl. In our case, $3\Delta l$ and $4\Delta l$ are used. The final result is obtained by taking the average of the solutions obtained for these two values. In order to illustrate this process, frequency spectra obtained with the TLM method for the two cases where c is equal to $10\Delta l$ are shown in Fig. 8. The solution obtained with the FD–TD method is also drawn in the same figure. As expected, the latter solution is located exactly between the two values obtained with the TLM method. This clearly illustrates the accuracy and convenience of the FD–TD method in such situations. Fig. 9 shows the dispersion characteristics of the microstrip which has the same cross section as that in Fig. 7. Again, both methods give very similar results except at higher frequencies, where the discretization errors associated with both methods become more pronounced, and their differences are more visible.

VII. CONCLUSIONS

The proposed new application of the FD–TD method to 3-D eigenvalue problems gives practically the same results

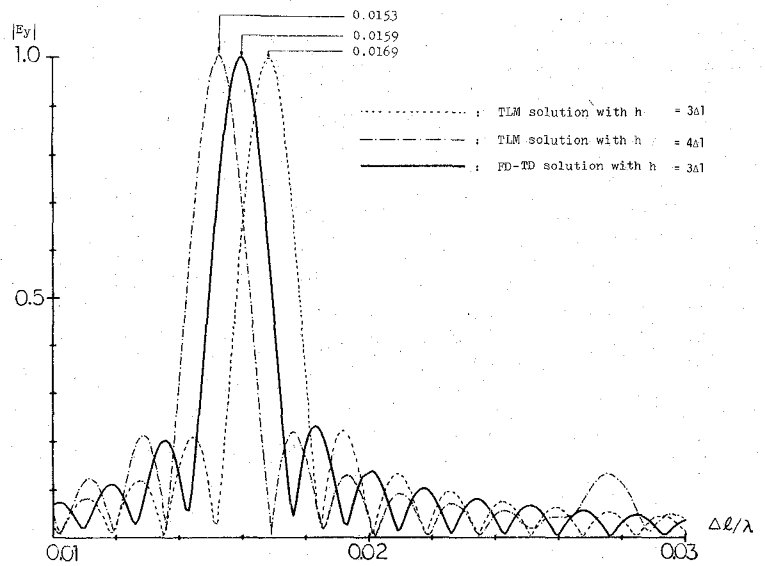

Fig. 8. Frequency spectra for the microstrip problem in Fig. 7, showing the effect of dielectric interface error in the TLM solution.

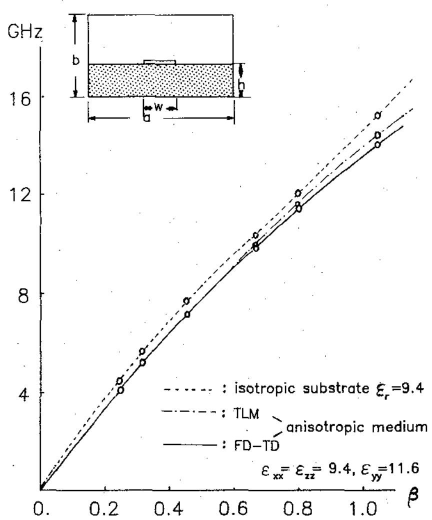

Fig. 9. Dispersion diagram of the anisotropic microstrip in Fig. 7.

as the TLM method under identical simulation conditions. However, the overall CPU time and storage requirements are typically less than half those needed in the TLM solution. Other advantages reside in the ease with which field distributions can be computed, and in the elimination of dielectric boundary error in planar structures. Further efforts are being made to implement losses, variable mesh size, and nonlinearity in the FD–TD procedure.

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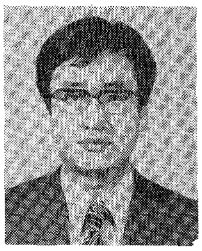

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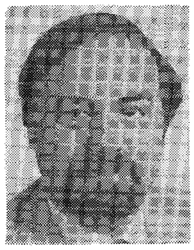

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