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# The Wave-Equation FD–TD Method for the Efficient Eigenvalue Analysis and S-Matrix Computation of Waveguide Structures

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***Abstract*—A new finite-difference time-domain (FD–TD) method is presented for the efficient computation of both the hybrid-mode eigenvalues and the scattering parameters of waveguide structures. The FD–TD formulation is based on the direct discretization of the vector wave equation, and requires advantageously only one grid (instead of two displaced grids in the commonly used curl equation approach). Moreover, merely the solution of three (instead of six) coupled equations is necessary. For 2D eigenvalue problems, the utilization of actual 2D grids and graded meshes yields a further reduction in the computational requirements, and, e.g., the whole dispersion characteristic (including evanescent modes) may be calculated very efficiently. For the *S*-parameter calculation, an excitation with a sinusoidally modulated Dirac impulse train is utilized. This combines the efficiency of frequency-domain methods with the flexibility of the standard FD–TD method. Typical numerical examples, such as the resonance frequencies for an inhomogeneously filled waveguide resonator, the hybrid-mode propagation characteristics of dielectric waveguiding structures, and the scattering parameters of the discontinuity of a dielectric slab of finite length in a rectangular waveguide, demonstrate the efficiency of the method. The theory is verified by comparison with results obtained by other methods.**

## I. Introduction

The finite-difference time-domain (FD–TD) method [1] is well established as a versatile numerical tool for solving the eigenvalues and scattering problems of a great variety of waveguiding structures [2]–[9]. One of the most attractive features of the method is its flexible applicability for structures with complicated circuit contours. On the other hand, however, a well-known drawback of the method in its standard formulation is the relatively large amount of memory space and CPU time required, in particular, for the full-wave analysis of hybrid mode waveguiding problems in inhomogeneous waveguiding structures. Several advances to reduce the mesh size for special waveguide problems have been reported in the past, therefore, ranging from the application of a two-dimensional FD–TD method for planar circuits [6] and a complex formulation for two-dimensional analysis problems [7], [8], to the formulation using nonorthogonal grids well appropriate for curvilinear structures [18].

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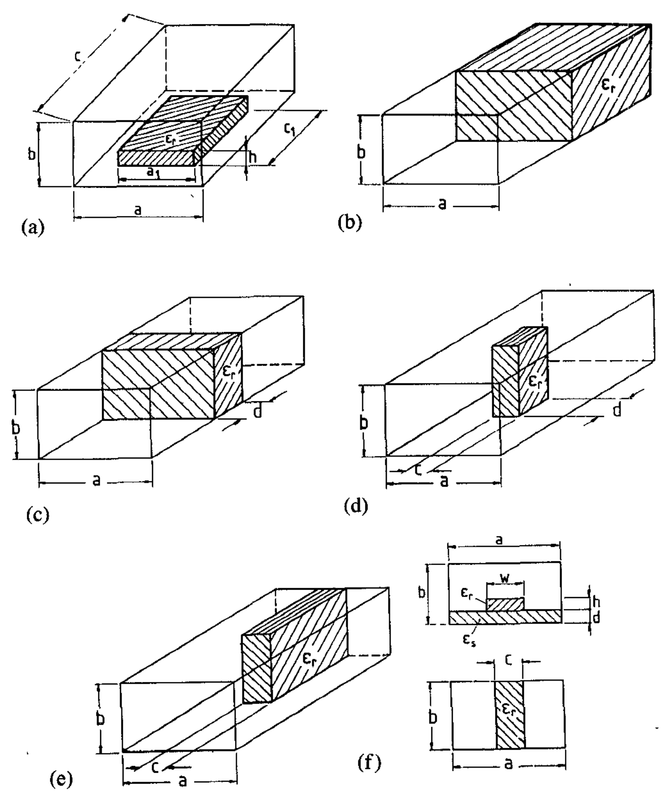


Fig. 1. Waveguide structures investigated with the FD–TD wave equation method. (a) Waveguide resonator. (b), (c) Step discontinuity of a waveguide filled with dielectric material. (d), (e) Step discontinuity of a dielectric slab in waveguide. (f) Insulated image guide and dielectric slab loaded waveguide.

In this paper, we utilize a different approach, the direct FD–TD wave equation discretization, which has, in particular, the advantage of reducing the numerical effort for both two- (2D) and three-dimensional (3D) waveguide problems. This formulation requires only one grid (instead of two displaced grids in the commonly used curl equation approach), and merely the solution of three (instead of six) coupled equations are necessary. For 2D eigenvalue problems, actual 2D grids are utilized [13] and a graded mesh algorithm is involved. This yields a further reduction in the computational requirements, and, e.g., the whole dispersion characteristic (including evanescent modes) may be calculated very efficiently. For scattering problems, an excitation with a sinusoidally modulated

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Dirac impulse train is utilized which combines the advantage of frequency-domain methods with the flexibility of the standard FD–TD method.

The efficiency of the method is demonstrated with typical examples. Numerical results are presented for the resonance frequencies for an inhomogeneously filled waveguide resonator, as well as for the fundamental—and higher order—mode propagation factors for the insulated image guide and the dielectric slab loaded waveguide. $S$-parameter calculation results are shown for a dielectric material loaded rectangular waveguide and for a dielectric slab of finite length in a rectangular waveguide (Fig. 1). The theory is verified by comparison with results obtained by other methods.

## II. Theory

The FD–TD method is usually formulated by discretizing Maxwell's curl equations over a finite volume and approximating the derivatives with centered difference approximations [1]–[8]. This leads to the three-dimensional Yee's mesh [1] in various modifications [2]–[5]. In this paper, we discretize directly the vector wave equation for inhomogeneous media

$$\mu\epsilon \frac{\partial^2 \vec{E}}{\partial t^2} = \nabla^2 \vec{E} - \nabla(\nabla \cdot \vec{E}) \tag{1}$$

which yields, in Cartesian coordinates (e.g., for $E_x$),

$$\frac{\partial^2 E_x}{\partial t^2} = \frac{1}{\epsilon\mu}\left[\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial^2 E_x}{\partial z^2} - \frac{\partial}{\partial x}\left(\frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}\right)\right]. \tag{2}$$

### A. Three-Dimensional FD–TD Wave Equation Formulation

Following Yee's notation, and assuming for simplicity a uniform discretization of (2), a reduced set of FD–TD equations for the electrical field is obtained where only the three electrical field components $E_x$, $E_y$, $E_z$ are coupled. We obtain, e.g., for $E_x$ [cf. Fig. 2(a)]

$$\begin{aligned} E_x^{n+1}(i, j, k) &= 2E_x^n(i, j, k) - E_x^{n-1}(i, j, k) \\ &+ \frac{s^2}{\epsilon_{rx}\mu_{rx}} \{E_x^n(i, j+1, k) - 2E_x^n(i, j, k) \\ &+ E_x^n(i, j-1, k) + E_x^n(i, j, k+1) - 2E_x^n(i, j, k) \\ &+ E_x^n(i, j, k-1) - \tfrac{1}{4}[E_y^n(i+1, j+1, k) \\ &- E_y^n(i+1, j-1, k) - E_y^n(i-1, j+1, k) \\ &+ E_y^n(i-1, j-1, k) + E_z^n(i+1, j, k+1) \\ &- E_z^n(i+1, j, k-1) - E_z^n(i-1, j, k+1) \\ &+ E_z^n(i-1, j, k-1)]\} \end{aligned} \tag{3}$$

where the stability factor is $s = c\Delta t/\Delta l$; $c$ is the velocity of light, and $\epsilon_{rx}$, $\mu_{rx}$ are the diagonal elements of the relative permittivity, or permeability tensor, respectively. The condition for stability in free space is $s \leq 1/\sqrt{3}$ [2]. The remaining finite difference equations related to the other two electric field equations can be similarly calcu-

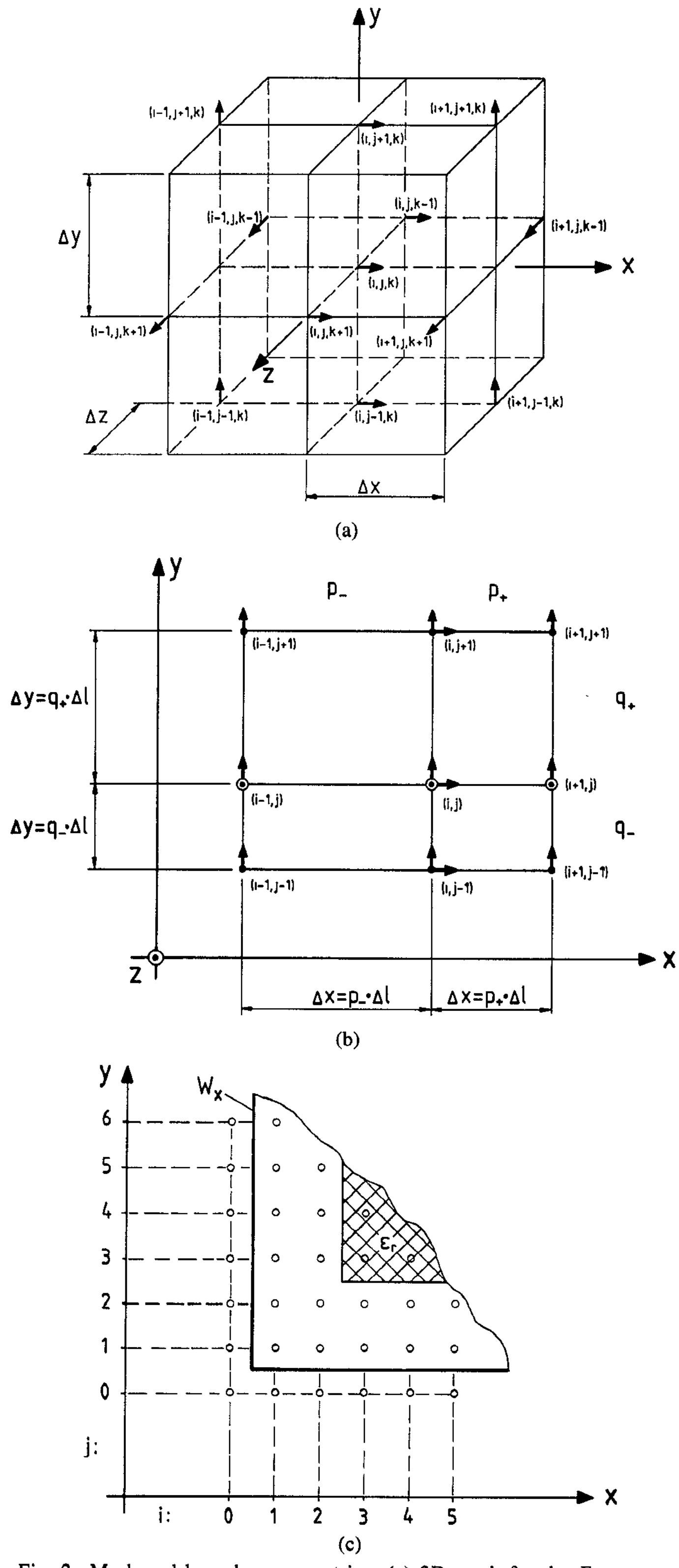


Fig. 2. Mesh and boundary geometries. (a) 3D mesh for the $E_x$ component. (b) Graded 2D mesh for the $E_x$ component. (c) Electric, magnetic, or absorbing boundary location.

lated. The magnetic field, if required, may easily be computed either in the time domain or, after solving for the electric field in the frequency domain, directly by using Maxwell's second equation.

### *B. Two-Dimensional FD–TD Wave Equation Graded Mesh Formulation*

A graded mesh in the $x$, $y$ direction [Fig. 2(b)] is an important feature to improve the computational efficiency of the FD–TD technique for 2D eigenvalue problems. Using the notation in Fig. 2(b), where $\Delta l$ is the smallest distance used in the mesh and $p$, $q$ are the graded mesh factors, the first- and second-order derivatives required in (2) may be written as follows:

$$\frac{\partial E(i,j)}{\partial x} = \frac{1}{\Delta l}\sum_{I=-1}^{1} c_x(I)\cdot E(i+I,j) \tag{4}$$

$$\frac{\partial E(i,j)}{\partial y} = \frac{1}{\Delta l}\sum_{J=-1}^{1} c_y(J)\cdot E(i,j+J) \tag{5}$$

$$\frac{\partial^2 E(i,j)}{\partial x^2} = \frac{1}{\Delta l^2}\sum_{I=-1}^{1} c_{xx}(I)\cdot E(i+I,j) \tag{6}$$

$$\frac{\partial^2 E(i,j)}{\partial y^2} = \frac{1}{\Delta l^2}\sum_{J=-1}^{1} c_{yy}(J)\cdot E(i,j+J) \tag{7}$$

$$\frac{\partial^2 E(i,j)}{\partial x\,\partial y} = \frac{1}{\Delta l^2}\sum_{I=-1}^{1}\sum_{J=-1}^{1} c_x(I)\cdot c_y(J)\cdot E(i+I,j+J) \tag{8}$$

with

$$c_x(-1) = -\frac{p_+}{p_-(p_-+p_+)},\quad c_x(0) = \frac{(p_+-p_-)}{p_-\cdot p_+},\quad c_x(1) = \frac{p_-}{p_+(p_-+p_+)}; \tag{9}$$

$$c_{xx}(-1) = \frac{2}{p_-(p_-+p_+)},\quad c_{xx}(0) = \frac{-2}{p_-p_+},\quad c_{xx}(1) = \frac{2}{p_+(p_-+p_+)} \tag{10}$$

and $c_y$, $c_{yy}$ are given analogously by the related graded mesh factor $q$.

For $z$-direction homogeneous structures, like in [7], [8], a complex notation is utilized, but in contrast to [7], [8], the phase factors $\gamma$ are directly introduced analytically, rather than using a uniform mesh extension of $\Delta l$ in the $z$-direction. This yields

$$\vec{E}(z) = \vec{E}(0)e^{-\gamma z};\quad \frac{\partial \vec{E}}{\partial z} = -\gamma\vec{E}(z);\quad \frac{\partial^2\vec{E}}{\partial z^2} = \gamma^2\vec{E}(z). \tag{11}$$

The two-dimensional formulation for, e.g., $E_x$ is then given by [cf. Fig. 2(b)]

$$\begin{aligned} E_x^{n+1}(i,j) = {} & 2E_x^n(i,j) - E_x^{n-1}(i,j) + \frac{s^2}{\epsilon_{rx}\mu_{rx}} \cdot \Bigg\{ \sum_{J=-1}^{1} c_{yy}(J)\cdot E_x^n(i,j+J) \\ & + \gamma^2\Delta l^2 E_x^n(i,j) - \sum_{I=-1}^{1}\sum_{J=-1}^{1} c_x(I) \cdot c_y(J)\cdot E_y^n(i+I,j+J) \\ & + \gamma\Delta l \sum_{I=-1}^{1} c_x(I)\cdot E_z^n(i+I,j)\Bigg\} \end{aligned} \tag{12}$$

where $s = (c\Delta t/\Delta l) \le 1/\{\sqrt{(2+(\beta_{\max}\Delta l/2)^2}\}$ according to [17].

### *C. Absorbing Boundary Conditions*

The electric wall, magnetic wall, and absorbing boundary conditions are assumed to be defined between two mesh nodes [cf. Fig. 2(c)]. The electric and magnetic walls are given in the usual way. Following [9], the FD–TD formulation of the absorbing boundary conditions for the region $x \ge 0$ in terms of the tangential electrical field components in the subregions (0) (outer region) and (1) (mesh region) may be written by

$$E_0^{n+1} = E_1^n + \frac{v_{px}\Delta t - \Delta x}{v_{px}\Delta t + \Delta x}(E_1^{n+1} - E_0^n) \tag{13}$$

where $v_{px}$ is the phase velocity in the $x$ direction. The formulations for $y$ and $z$ are found analogously.

### *D. Eigenvalue Calculation Procedure*

The principal numerical calculation steps for both 3D and 2D problems are similar to those in the conventional FD–TD approach. For 2D problems, however, a phase factor $\gamma$ has to be selected first. Note that the selection of the related phase factor $\gamma = \alpha$ yields the possibility of also calculating the evanescent portion of the dispersion diagram. After placing the appropriate boundary conditions, launching an excitation pulse, waiting until the distribution of the pulse is stable, and performing the Fourier transformation, the modal frequencies related to the selected propagation factor are obtained.

### *E. S-Parameter Calculation Procedure*

The discontinuity under consideration is divided in the usual way [12], [14] into the areas: 1) discontinuity region, and 2) longitudinally homogeneous waveguiding structures attached to the discontinuity as the input and output ports. For the $S$-parameter calculation, the structure to be investigated is discretized in the same manner as in the case of the eigenvalue calculation, but a new excitation is employed, like for the FD–TLM method in [12], which is a sinusoidally modulated Dirac impulse train. This method combines both the flexibility of the conventional FD–TD method and the computational efficiency of frequency-domain techniques. The excitation waveform may also be regarded as a continuous sinusoidal wave sampled at discrete time values. This approach allows one to transform the FD–TD solution procedure directly into the frequency domain. The method is particularly useful for dispersive structures for which the required frequency-dependent absorbing boundaries may conveniently be simulated by (13) by using frequency- and mode-dependent propagation velocities.

The first step in the $S$-parameter calculation is the solution of the cross-section eigenvalue problem for the chosen input and output waveguide structure under consideration. This yields the necessary dispersion characteristics (also for the absorbing boundary simulation) and cross-section field distribution for the propagating modes. If the position of the absorbing boundaries and the input and output waveguides are chosen so that merely the fundamental mode propagates there; the influence of the higher order modes in the input and output waveguides can be neglected. The selected input port is then (second step) excited by its modal (in our case, fundamental mode) field distribution which is sinusoidally modulated. After an appropriate number of time iterations, a stable distribution is obtained, and the DFT algorithm can be applied in order to yield the desired complex field amplitude coefficients at the corresponding frequency.

In a third step, similar to the procedure described in [14], the magnitude and phase of the mode amplitudes $a_i$ and $b_i$ are determined by calculation of the modal power relation

$$\sqrt{\int_A \vec{E}_t \times \vec{H}_{ti} \cdot d\vec{A}} = a_i(z) + b_i(z) \qquad (14)$$

at two different planes $z_p$ and $z_p + n\Delta z$, where $E_t$, $H_{ti}$ are the complete electric and modal magnetic fields, respectively. The relations simplify if only the fundamental mode in the input and output waveguides is considered. Moreover, the usual expressions for uniform waveguides may advantageously be utilized [15]. The relations

$$a_i(z_p + \Delta z) = a_i(z_p) \cdot e^{-\gamma_i(\Delta z)},$$
$$b_i(z_p + \Delta z) = b_i(z_p) \cdot e^{+\gamma_i(\Delta z)} \qquad (15)$$

are used to obtain the mode amplitudes $a_i$ and $b_i$ since $\gamma$ in the input and output waveguides is known.

## III. Results

Good agreement between the results of the FD–TD wave equation method for a 3D eigenvalue problem and those calculated by the standard FD–TD and TLM method (own calculations) are demonstrated for the example of a waveguide resonator inhomogeneously filled with dielectric, Fig. 3. For all calculations, the same discretization

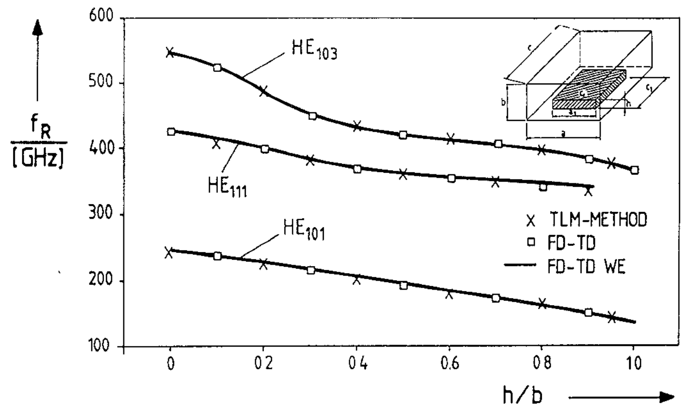


Fig. 3. Waveguide resonator inhomogeneously filled with dielectric. $a_1 = c_1 = b$. Discretization: 10 × 10 × 10. Number of time iterations $N_t = 2000$. $\epsilon_r = 4$, WR-3 waveguide.

(10 × 10 × 10) and number of time iterations ($N_i = 2000$) is used without any filtering or spectrum estimation techniques. The CPU time for the FD–TD wave equation method is less by about 30% as compared with the standard FD–TD method. A further check of the accuracy was carried out for the simple empty resonator of Fig. 3 by comparison with the results obtained with analytical formulas for the resonant frequency. Although the discretization was relatively coarse ($\Delta l = b/10$), the error was less than 1%.

For a dispersion diagram of a waveguide structure with hybrid modes, a comparison with results of the 2D FD–TD method of [8] and of the FD–FD method of [10] is presented in Fig. 4 at the example of the propagation factor for the shielded insulated image guide. Very good agreement may be stated. The CPU time saving of the FD–TD wave equation method as compared with the already efficient 2D FD–TD method of [8] is about 30%.

Fig. 5 shows the magnitude of the input reflection coefficient for a transition empty rectangular waveguide to an infinitely long waveguide homogeneously filled with dielectric material as a function of the permittivity $\epsilon_r$ for different frequencies. In this case, analytical solutions are available; cf. [12]. Very good agreement with those values may be stated. The same is true for the structure of finite length $d$, Fig. 6, where the magnitudes of the presented FD–TD wave equation method (solid lines) are in very good agreement with the scattering parameter calculations carried out by using the classical 3D FD–TD method requiring the solution of six coupled equations.

The transition rectangular waveguide to dielectric slab loaded waveguide is treated in Fig. 7. First, the whole dispersion diagram for the fundamental mode is calculated, including the evanescent part, Fig. 7(a). The results (solid lines) are in very good agreement with the standard 2D FD–TD method (Δ Δ Δ); moreover, the calculated phase factor for the $TE_{10}$ mode in the rectangular waveguide section is identical with the analytical result (□ □ □). For the calculation of the input reflection coefficient, an appropriate absorbing boundary has been placed in the dielectric slab loaded waveguide section by using

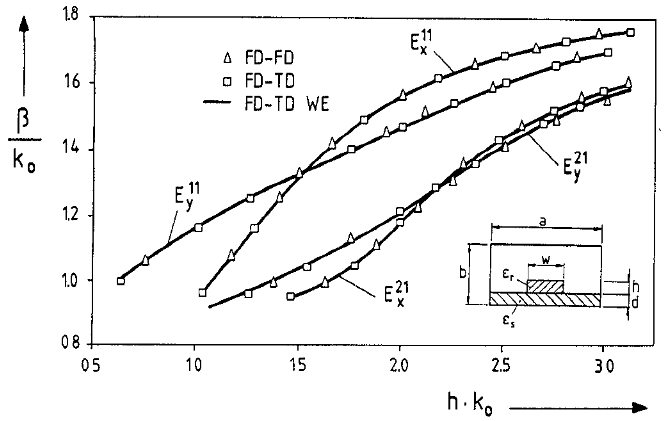


Fig. 4. Shielded insulated image guide. $w/h = 2.25$, $d/h = 0.5$, $a/h = 13.5$, $b/h = 8$, $\epsilon_r = 3.8$, $\epsilon_s = 1.5$. Discretization: 54 × 64. Number of times iterations $N_t = 1000$.

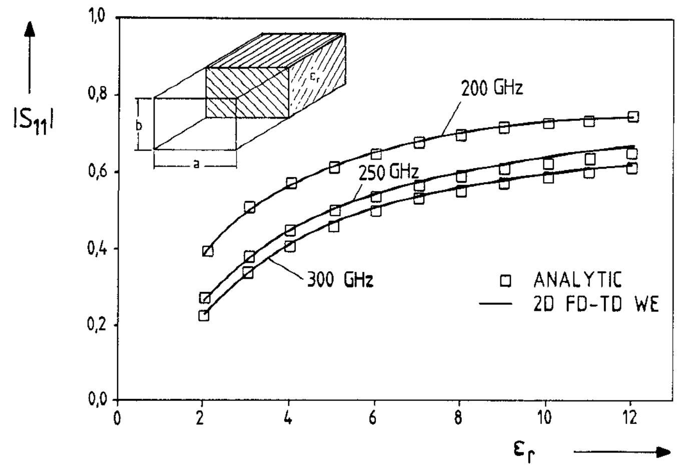


Fig. 5. Input reflection coefficient for a transition rectangular waveguide to infinitely long waveguide homogeneously filled with dielectric material as a function of the permittivity $\epsilon_r$ for different frequencies. Comparison with analytically calculated values (□ □ □). WR-3 housing, discretization: 50 × 10, number $N_t$ of time iterations $N_t = 2000$.

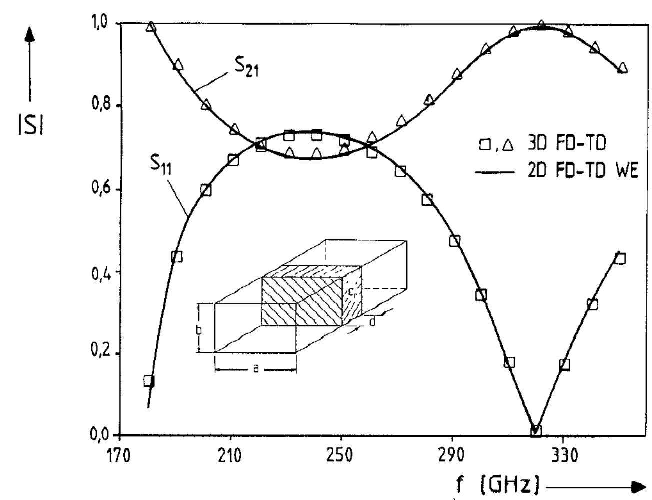


Fig. 6. Scattering parameters for the step discontinuity rectangular waveguide to waveguide homogeneously filled with dielectric material of finite length $d$. Comparison of the results FD-TD wave equation method (solid lines) with scattering parameter calculations by using the classical 3D FD-TD method (□ □ □, Δ Δ Δ). $\epsilon_r = 3.7$, WR-3, $d = 0.504$ mm. Discretization: 12 × 64; 12 × 12 × 90; $N_t = 2000$.

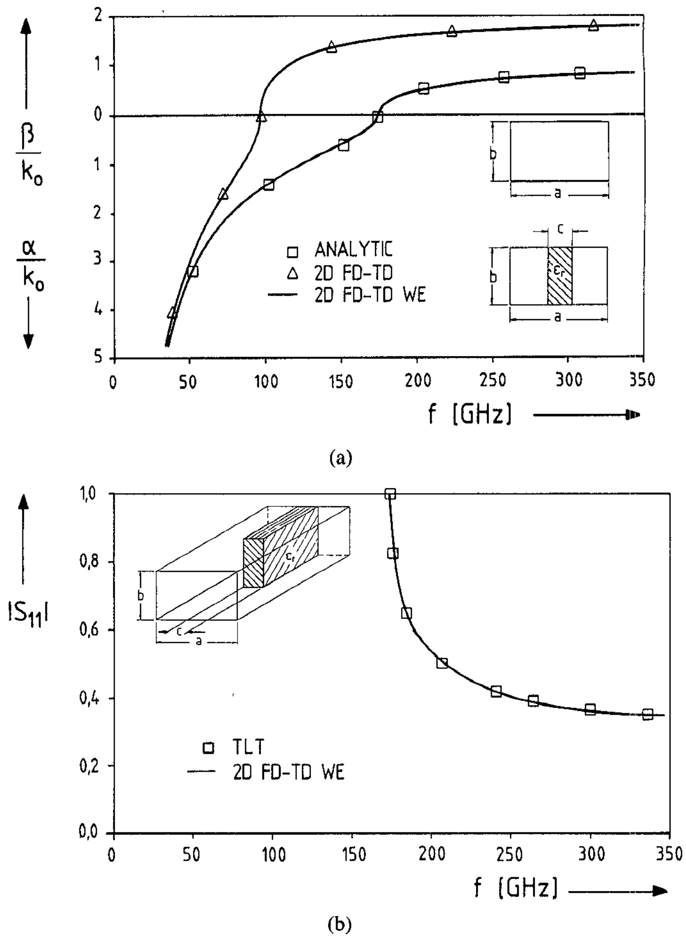


Fig. 7. Dielectric slab loaded waveguide. (a) Dispersion diagram for the fundamental mode in both sections. Comparison with the standard 2D FD-TD method (Δ Δ Δ) and the analytical solution (rectangular waveguide section) (□ □ □). (b) Input reflection coefficient. Comparison with results by using the transmission line (TLT) relations for longitudinally homogeneous waveguides [15]. WR-3, $c = a/2$, $\epsilon_r = 3.7$, $N_t = 2000$, discretization: 90 × 16.

the relations [13], together with the appropriate frequency-dependent expression for the phase velocities. The results [Fig. 7(b)] are in close agreement with results obtained by using the transmission line (TLT) relations for longitudinally homogeneous waveguides [15].

Fig. 8 presents the investigation of the transition rectangular waveguide to the dielectric slab loaded waveguide of finite length. The input reflection coefficient calculated by the presented FD-TD wave equation method for two distinct numbers $N_i$ of time iterations is compared with measurements [16] performed in the $X$ band. A continuously graded symmetric mesh in the $z$ direction has been used with a finer mesh size in the region of the dielectric slab. Although a relatively low number of discretization steps (50 × 15) are chosen and the standard Mur's absorbing boundaries have been placed rather closely to the discontinuity (the distance is only about $\lambda_g/3$ at the lowest frequency), excellent agreement with measurements may be stated; cf. the solid curve in Fig. 8. The number $N_t$ of time iterations required for good results is, however, relatively high; cf. the solid curve (for $N_i$ =

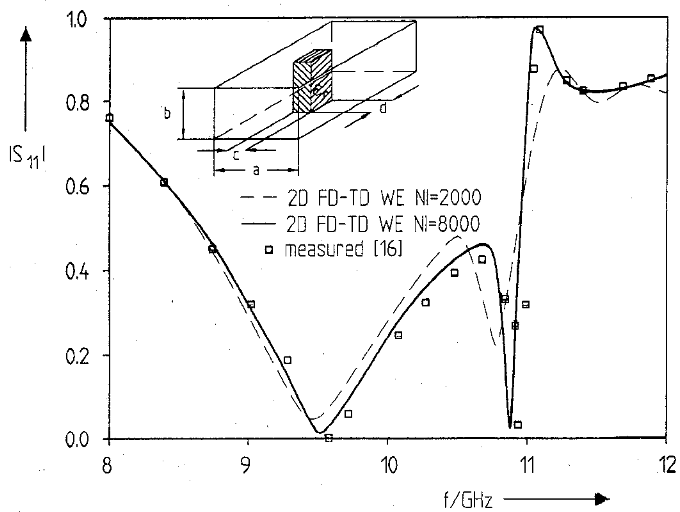


Fig. 8. Dielectric slab loaded waveguide of finite length. Reflection coefficient of the transition rectangular waveguide to dielectric slab loaded waveguide of finite length. Comparison with measurements [16]. $a = 22.86$ mm, $b = 10.16$ mm, $c = 12$ mm, $d = 6$ mm, $\epsilon_r = 8.2$, discretization: 50 × 15.

8000) in comparison with the dashed curve (for $N_i = 2000$).

## IV. Conclusion

An efficient full-wave FD–TD formulation based on the direct discretization of the vector wave-equation is proposed for the accurate analysis of 2D and 3D waveguiding structures. For this formulation, only one grid is required instead of the two displaced grids of the usual approach, and merely the solution of three coupled equations instead of six is necessary. For the *S*-parameter calculation, an excitation with a sinusoidally modulated Dirac impulse train is utilized which combines the efficiency of frequency-domain methods with the flexibility of the standard FD–TD method. The theory is verified by comparison with results obtained by other methods.

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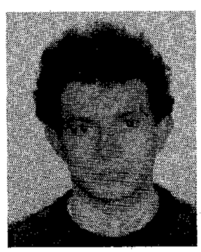

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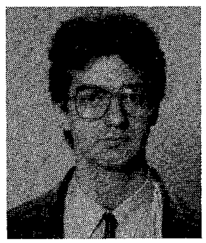

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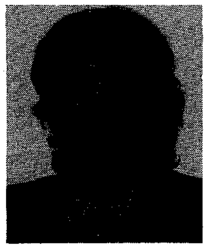

**Fritz Arndt** (SM'83–F'93) received the Dipl.-Ing. Dr.-Ing., and Habilitation degrees from the Technical University of Darmstadt, Germany in 1963, 1968, and 1972, respectively.

From 1963 to 1972 he worked on directional couplers and microstrip techniques at the Technical University of Darmstadt. Since 1972 he has been a Professor and head of the Microwave Department of the University of Bremen, Germany. His research activities are in the area of the solution of field problems of waveguide, finline, and optical waveguide structures, of antenna design, and of scattering structures.

Dr. Arndt is a member of the VDE and NTG (Germany). He received the NTG Award in 1970, the A. F. Bulgin Award (together with three coauthors) from the institution of Radio and Electronic Engineers in 1983, and the Best Paper Award of the Antenna Conference JINA 1986 (France).