Efficient FDTD/Matrix-Pencil Method for the Full-Wave Scattering Parameter Analysis of Waveguiding Structures

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***Abstract*— A combined finite-difference time-domain/matrix-pencil method is presented for the efficient and rigorous calculation of the full-wave modal S-parameters of waveguide components including structures of more general shape or high complexity. The application of the S-parameter definition for unmatched ports requires merely standard Mur's absorbing boundaries for reliable results, and a nonorthogonal or contour path mesh formulation allows the convenient inclusion of curved boundaries. The efficiency of the method is demonstrated at the analysis of waveguide and monolithic microwave millimeter wave integrated circuit (MMIC) components of practical importance, such as the twisted waveguide, the twisted waveguide bend, the post compensated magic T, the waffle-iron filter, and the MMIC spiral inductor including an air bridge. The method is verified by excellent agreement with measurements, with finite element method (FEM) or moment method results.**

I. Introduction

The advanced design of waveguide components is increasingly based on rigorous field theory methods [1]–[12]. Many common elements which are compatible with the Cartesian or cylindrical coordinate systems can be simulated directly with the efficient mode-matching method [1]–[4]. However, there is growing interest in structures of more general shape. These offer, for instance, the advantage of more compact size, such as twisted bends, or the potential of improved designs by additional design parameters, such as the partial height post compensated magic T. Appropriate CAD methods for such structures are therefore very desirable.

Several different techniques have already been applied so far. Miter compensated T-junctions are investigated by a finite element method (FEM) in [5]. A boundary-contour mode-matching method [6] has been used for a class of arbitrarily shaped H- and E-plane discontinuities. Due to its high flexibility, however, the finite-difference time-domain (FDTD) method is considered to be particularly well applicable for more complex waveguiding structures.

Typical waveguide elements hitherto investigated by the FDTD method are inductive irises or inductive iris filters [7], [9], transitions and T-junctions [8], H-plane couplers [10], H-plane corners with inductive posts [11], and cylindrical cavities [12]. It indicates that mostly step type structures have been analyzed so far (which have been calculated also by the mode matching technique before). This seems to be mainly due to well-known problems in the usual FDTD simulation of waveguide elements. These are typically the large number of required time steps, the existence of resonant cavities, the lack of general and efficient absorbing boundaries, the lack of adequate S-parameter extraction techniques also for higher-order modes, as well as the occurrence of curvilinear structures. Resonant cavities, in particular, require a long time response which leads—in combination with convolution-type absorbing boundary conditions—to a very high computational effort.

This paper presents an improved FDTD technique which allows the very efficient full-wave modal S-matrix calculation of a comprehensive class of general waveguide structures, such as twisted bends, post compensated magic T's, and waffle-iron filters (Fig. 1). Moreover, the convenient applicability of the presented technique also to the scattering parameter calculation of more complex monolithic microwave millimeter wave integrated circuit (MMIC) structures is demonstrated at the example of a spiral inductor with an air-bridge (Fig. 1).

Typical problems occurring in the usual FDTD simulation of waveguide elements are solved successfully by adequate techniques.

1) In order to reduce the high computational effort resulting from the usually required large number of time steps, the efficient matrix pencil technique [13] is utilized. This technique needs less CPU time and is less sensitive to noise influences than, for instance, the often used Prony's method [14], [12].
2) The application of the modal S-parameter definition for unmatched ports [29] achieves even with standard Mur's absorbing boundaries excellent and reliable results.
3) A structure dependent mesh is used based on nonorthogonal [15] or contour path grid cells [16], respectively, according to the specific form of the boundary.

II. Theory

The powerful combination of the FDTD method for Maxwell's equations [15]–[17] (or in its vector wave equation form [18]) and the matrix pencil technique [13] is used for the full-wave analysis waveguide structures of more general shape. This technique avoids the drawbacks of the slow convergence of the standard fast Fourier transform (FFT) formulation, and of the very small time increments, when applied to structures

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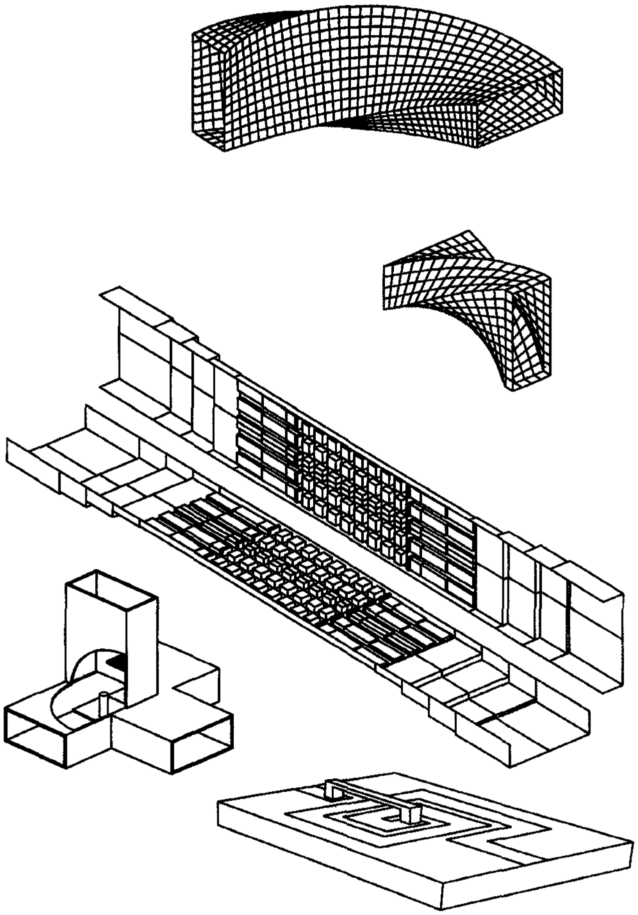

Fig. 1. Typical structures investigated with the improved FDTD technique: Twisted 90° bend, compensated magic T, waffle-iron filter, MMIC spiral inductor.

which are small compared with the wavelength. Since the basics of the FDTD formulation are well known, only the additional aspects, utilization of the matrix pencil method and the generalized S-matrix technique, are treated in more detail.

A. Matrix Pencil Technique

Like for Prony's method [14], [19], [20], the time transient wave form is approximated for the matrix pencil technique [13], [21], [22] by a sum of damped complex exponentials

$$\begin{aligned} y_k &= x_k + n_k \\ &= \sum_{t=1}^{M} |b_t| e^{(\alpha_t + j\omega_t)k + j\phi_t} + n_k \\ &= \sum_{t=1}^{M} b_t z_t^k + n_k \end{aligned} \tag{1}$$

where $k = 0, 1, \cdots, N-1$ is the time index, n_k indicates additional noise. The $z_t = e^{\alpha_t + j\omega_t}$ are the poles, and $b_t = |b_t| e^{j\phi_t}$ denote the residuals of the noiseless time signal x. The basic idea of the matrix pencil method, and the significant difference in comparison with Prony's method, is to formulate an eigenvalue problem for the determination of the poles z_t, $t = 1, \cdots, M$.

With the data vectors $\boldsymbol{x}_t$ of length $N - L$ for the noiseless signal x_k

$$\boldsymbol{x}_t = [x_t, x_{t+1}, \cdots, x_{N-L+t-1}]^T. \tag{2}$$

The matrices X_0 and X_1 are defined

$$X_{0(N-L)\times L} = [\boldsymbol{x}_{L-1}, \boldsymbol{x}_{L-2}, \cdots, \boldsymbol{x}_0] \tag{3}$$

$$X_{1(N-L)\times L} = [\boldsymbol{x}_L, \boldsymbol{x}_{L-1}, \cdots, \boldsymbol{x}_1]. \tag{4}$$

Every pole z_t, $t = 1, \cdots, M$ reduces the rank of the "matrix-pencil" $X_1 - z_t X_0$ exactly by one [13], if the "pencil-parameter" L is chosen to be $M \le L \le N - M$; in this case, the matrix-pencil $X_1 - z_t X_0$ is of rank $M - 1$. Otherwise, the rank of the matrix-pencils remains M. This means, that each pole is an eigenvalue of the generalized eigenvalue problem

$$(X_1 - z_t X_0)\boldsymbol{q}_t = 0 \tag{5}$$

with nonquadratic matrices, if L is chosen to be $M \le L \le N - M$. Equation (5) is transformed into a standard eigenvalue problem of a quadratic matrix by multiplication from left with the pseudo inverse [23] X_0^+ of the matrix X_0

$$(X_0^+ X_1 - z_t I)\boldsymbol{q}_t = 0 \tag{6}$$

which does not change the eigenvalues and -vectors. With (6), the z_t are exactly the M nonzero eigenvalues of the matrix $X_0^+ X_1$. Since the matrix $X_0^+ X_1$ is of rank M, there are additional $L - M$ zero eigenvalues.

For the noisy signal, analogously to X_0, X_1, the matrices Y_0, Y_1 are defined, and the eigenvalue problem can be formulated in the same way as in (5). In contrast to the noiseless case, the data matrices Y_0, Y_1 might have the full rank $P = \min(N - L, L)$ even if the signal contains only $M < P$ poles. Therefore the transformation of the matrix-pencil into a standard eigenvalue problem of a matrix of rank M is performed by the multiplication with the "truncated pseudo inverse matrix" Y_0^+ [23]. To obtain an estimation of the number of poles M of the noisy signal and to compute the truncated pseudo inverse of the noisy data matrix Y, a singular value decomposition (SVD) [25] $Y_0 = U\Sigma V^H$ is carried out, wherein Σ is a diagonal matrix containing the singular values, and U, V are the corresponding orthogonal basis vectors of the mapping- and the null space. The pseudo inverse can be expressed by the matrices of the SVD: with the SVD of an arbitrarily complex matrix A of the rank $\mathrm{Rk}(D)$, $A = U\Sigma V^H$, $\Sigma = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix}$, where pseudo inverse is defined as $A^+ = VD^{-1}U^H$ [23].

For the computation of the truncated pseudo inverse, only the M largest singular values in the diagonal matrix Σ are used; all other elements are set to zero, so that the resulting truncated pseudo inverse matrix is of rank M. For the calculated examples, the limit for the lowest considered singular value σ_M has been chosen to be $\sigma_1 \cdot 10^{-6}$ (where σ_1 is the largest singular value), which determines the number of the poles M. Because the corresponding rows of the matrix V and columns of the matrix U^H related to the zero diagonal elements of Σ do not contribute to the pseudo inverse, the

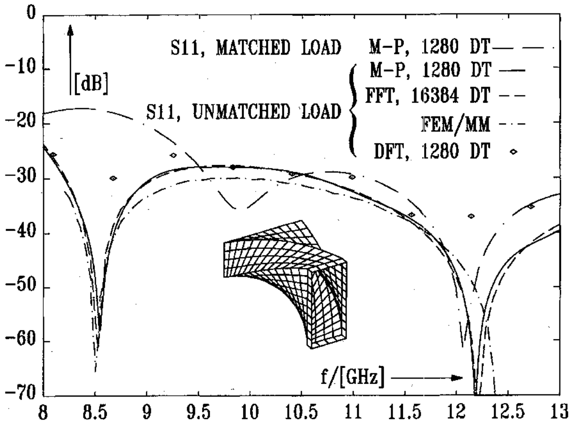

Fig. 2. Return loss of a 90° twisted rectangular X-band waveguide. FDTD-Matrix-Pencil-method, 1280 Δt (——), comparison with FDTD-FFT for 16 384 Δt (- - -), FEM/MM results (- · - ·), FDTD-DFT results (◊ ◊) for 1280 Δt and the standard matched-load S-parameter extraction procedure (· - - ·). Dimensions: WR90 waveguide, 22.86 × 10.16 mm, length of the twisted region: 31.75 mm. Applied discretization: 38 × 17 × 104 cells.

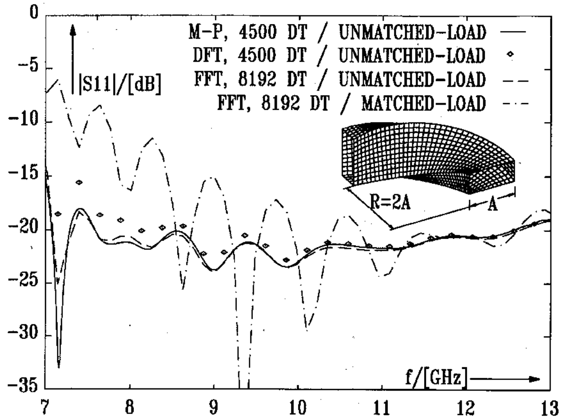

Fig. 3. Return loss of a 90° twisted 90°-bend, obtained with FDTD matrix-pencil-method, 4500 Δt (——), compared with FDTD-FFT results for 16 384 Δt (- - -), FDTD-DFT results for 4500 Δt (◊ ◊), and FDTD-FFT results (· - - ·) utilizing the matched-load S-parameter extraction procedure. Dimensions: WR90 waveguide, $A = 22.86 \times 10.16$ mm, bend-radius: $2A$. Discretization: 34 × 16 × 202 cells.

dimensions of these matrices are reduced accordingly, and the reduced matrices designated with V_0 and U_0^H, respectively.

In the corresponding eigenvalue problem which is analogous to (6)

$$Y_0^+ Y_1 \boldsymbol{q}_t = z_t \boldsymbol{q}_t \tag{7}$$

the truncated pseudo inverse Y_0^+ is given by the reduced matrices of the SVD $Y_0^+ = V_0 D^{-1} U_0^H$, which results in

$$V_0 D^{-1} U_0^H Y_1 \boldsymbol{q}_t = z_t \boldsymbol{q}_t. \tag{8}$$

Because $V_0^H V_0 = I_M$ and $\boldsymbol{q}_t = V_0^H V_0 \boldsymbol{q}_t$, the multiplication of (8) from left with V_0^H leads to

$$D^{-1} U_0^H Y_1 V_0 (V_0^H \boldsymbol{q}_t) = z_t (V_0^H \boldsymbol{q}_t). \tag{9}$$

The eigenvalues z_t are determined by the eigenvalue problem for the asymmetric $M \times M$ matrix

$$Z_E = D^{-1} U_0^H Y_1 V_0. \tag{10}$$

With the then known poles z_t, the residuals b_i are immediately given by the solution of the least squares problem

$$\min_b \|Z_N \boldsymbol{b} - \boldsymbol{y}\|, \quad \text{with} \tag{11}$$

$$Z_N = \begin{bmatrix} z_1^0 & z_2^0 & \cdots & z_M^0 \\ z_1^1 & z_2^1 & \cdots & z_M^1 \\ & & \cdots & \\ z_1^{N-1} & z_2^{N-1} & \cdots & z_M^{N-1} \end{bmatrix}$$

which requires merely the SVD of the matrix Z_N.

For the application of the matrix pencil technique to FDTD-time signals, first the number of signal poles at the calculation of the pseudo inverse matrix Y_0^+ is determined by the chosen minimum value of $\sigma_M \geq \sigma_1 \cdot 10^{-6}$.

Since the FDTD time signals are very oversampled, only every $(N_{\text{skip}} + 1)$th value is considered for the matrix pencil formulation. This undersampling is usually determined by the maximum frequency of interest.[1] Generally, N_{skip} has to be selected so that the estimated number of poles M is less than the half of the totally involved time steps N_{MP}.

The spectrum of the time signal can now be expressed in terms of poles and residues according to

$$F(\omega) = \sum_{s=-\infty}^{\infty} \sum_{t=1}^{M} \frac{b_t}{j(\omega + s\omega_{\max} - \omega_t) - \alpha_t} + C \tag{12}$$

where $\omega_{\max} = \frac{2\pi}{\Delta t}$ denotes the spectral period, Δt is the timestep of the undersampled signal and C is a constant resulting from a DIRAC-impulse in the time-signal at $t = 0$.[2]

Due to the undersampling of the time-signal and the fact that a pole represents an infinite spectrum, in practice, a large number of spectral periods have to be taken into account to obtain a convergent value for $F(\omega)$. Especially poles with large attenuation constants, representing the very short portions of the time signal, cause the slow convergence behavior of $F(\omega)$. Therefore these poles are isolated from the sum in (12). Because of their fast converging time domain representation they are transformed separately to the frequency domain by a DFT.

B. Modal S-Parameter Extraction

In order to obtain accurate results even when using standard first order absorbing boundary conditions, the unmatched port S-parameter definition [29] is applied, where in the case of a general N-port discontinuity, one has to consider a system of N equations in the form

$$B = SA \tag{13}$$

where $B = (\boldsymbol{b}_1, \boldsymbol{b}_2, \cdots, \boldsymbol{b}_N)$ is a matrix formed by N different $\boldsymbol{b}$-vectors and $A = (\boldsymbol{a}_1, \boldsymbol{a}_2, \cdots, \boldsymbol{a}_N)$ is a matrix formed by N different $\boldsymbol{a}$-vectors. The desired modal S-matrix is obtained by

[1] This may require a preceeding lowpass filtering of the original FDTD signal.

[2] y_n can be expressed by the sum of an even and an odd function plus $\delta_n y_n \frac{1}{2}$ where $\delta_n = 1 \Leftrightarrow n = 0$, $\delta_n = 0 \Leftrightarrow n \neq 0$.

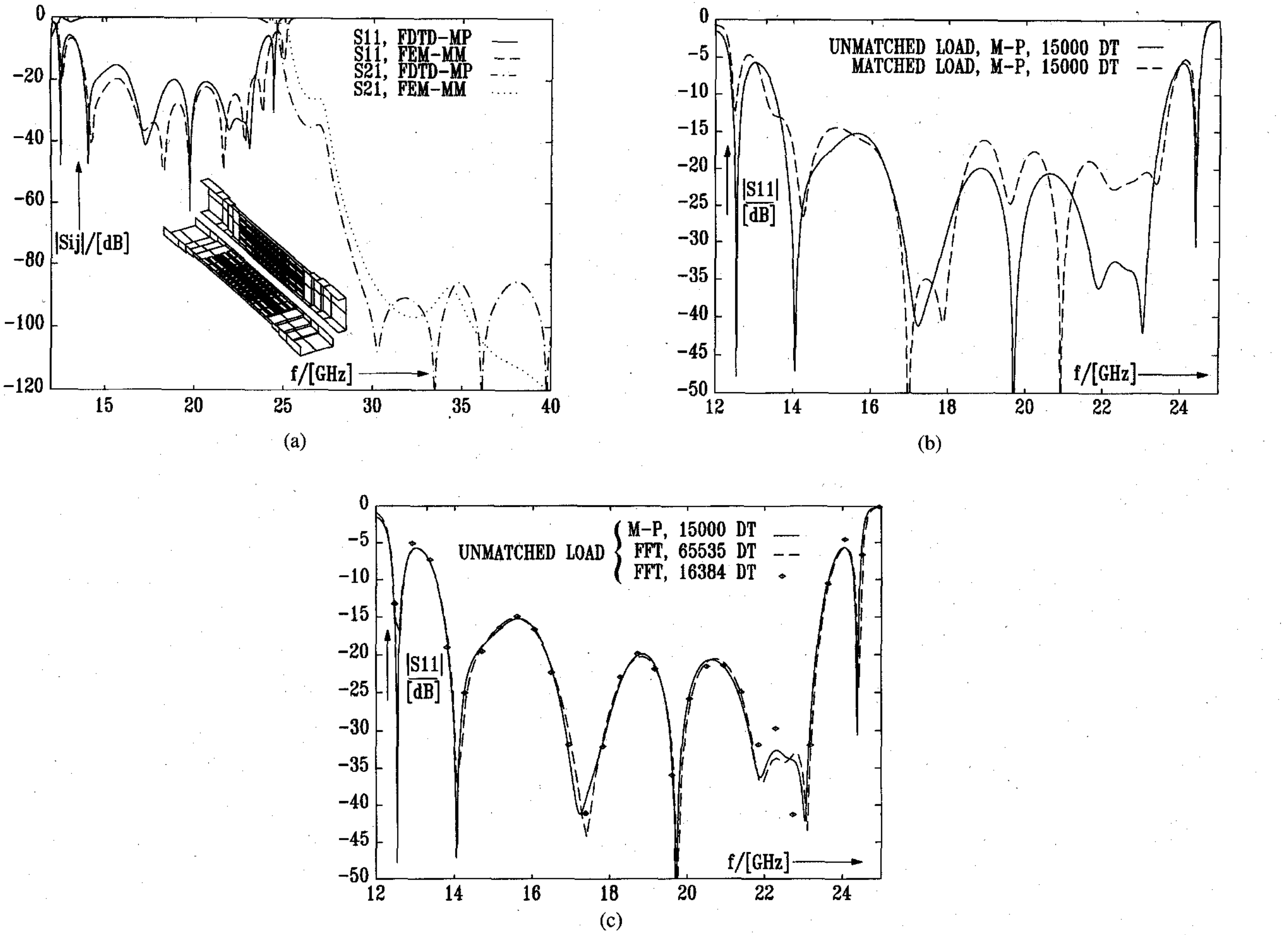

Fig. 4. Waffle-iron filter of Matthaei, Young, Jones. (a) Verification of the FDTD-matrix-pencil results (——), (- · - ·) with the FE/MM method (- - -), (· · · ·). (b) Comparison with the standard matched load approach (- - -) , (65 535 timesteps) and (◊ ◊), (16 384 timesteps). Dimensions: see [28]. Discretization: 710 060 cells in nine grids.

the multiplication of (13) with the inverse of matrix A, from the right side.

The N different vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, respectively, are calculated by N appropriate simulation runs, each considering a different condition, e.g., the excitation of a different port. If more then one mode is present on a port of the structure under investigation, an extraction of the modal guided power has to be performed. For that purpose, we use the orthogonal mode properties similar to [24]. The required modal field distribution can be obtained by using the compact 2-D FDTD approach [26], or by analytical formulations in the case of rectangular, circular, or elliptic waveguide ports.

The transversal electric field $\vec{E}_t^j$-obtained by the three-dimensional (3-D) FDTD method at the position z of port j can be written in the form

$$\vec{E}_t^j(z) = \sum_{p=1}^{M} \vec{e}_{tp}^{\,j}(a_p^j \cdot e^{-\gamma_p z} + b_p^j \cdot e^{+\gamma_p z}) \tag{14}$$

where $\vec{e}_{tp}^{\,j}$ is the transversal field distribution of the electric field of the mode p at port j, and a_p^j, b_p^j are the modal amplitudes. With $\vec{\boldsymbol{h}}_{tq}^j$ representing the transversal magnetic field distribution of the mode q at the same port, the following integration along the cross section A_j of port j has to be performed

$$\begin{aligned}\frac{1}{d_q}\iint_{A_j} \vec{E}_t^j(z) \times \vec{\boldsymbol{h}}_{tq}^j \, dV_2 &= a_q^j \cdot e^{-\gamma_q z} + b_q^j \cdot e^{+\gamma_q z} \\ &= w_q^j(z).\end{aligned} \tag{15}$$

The normalization constant d_q is calculated from the modal field distributions $\vec{e}_{tq}^{\,j}$ and $\vec{\boldsymbol{h}}_{tq}^j$, by the following equation

$$d_q = \iint_{A_j} \vec{e}_{tq}^{\,j} \times \vec{\boldsymbol{h}}_{tq}^j \, dV_2. \tag{16}$$

Since the propagation constant γ of each mode is also obtained by the 2-D FDTD calculation step or analytically known, the incident and scattered modal amplitudes a_q^j, b_q^j can be determined by the following two equations involving the evaluation of (15) at two cross sections $z = 0$ and $z = \Delta z$ of port j

$$a_q^j = \frac{w_q^j(z) - w_q^j(z+\Delta z)e^{-\gamma_q \Delta z}}{1 - e^{-2\gamma_q \Delta z}} \tag{17}$$

$$b_q^j = \frac{w_q^j(z) - w_q^j(z+\Delta z)e^{+\gamma_q \Delta z}}{1 - e^{+2\gamma_q \Delta z}}. \tag{18}$$

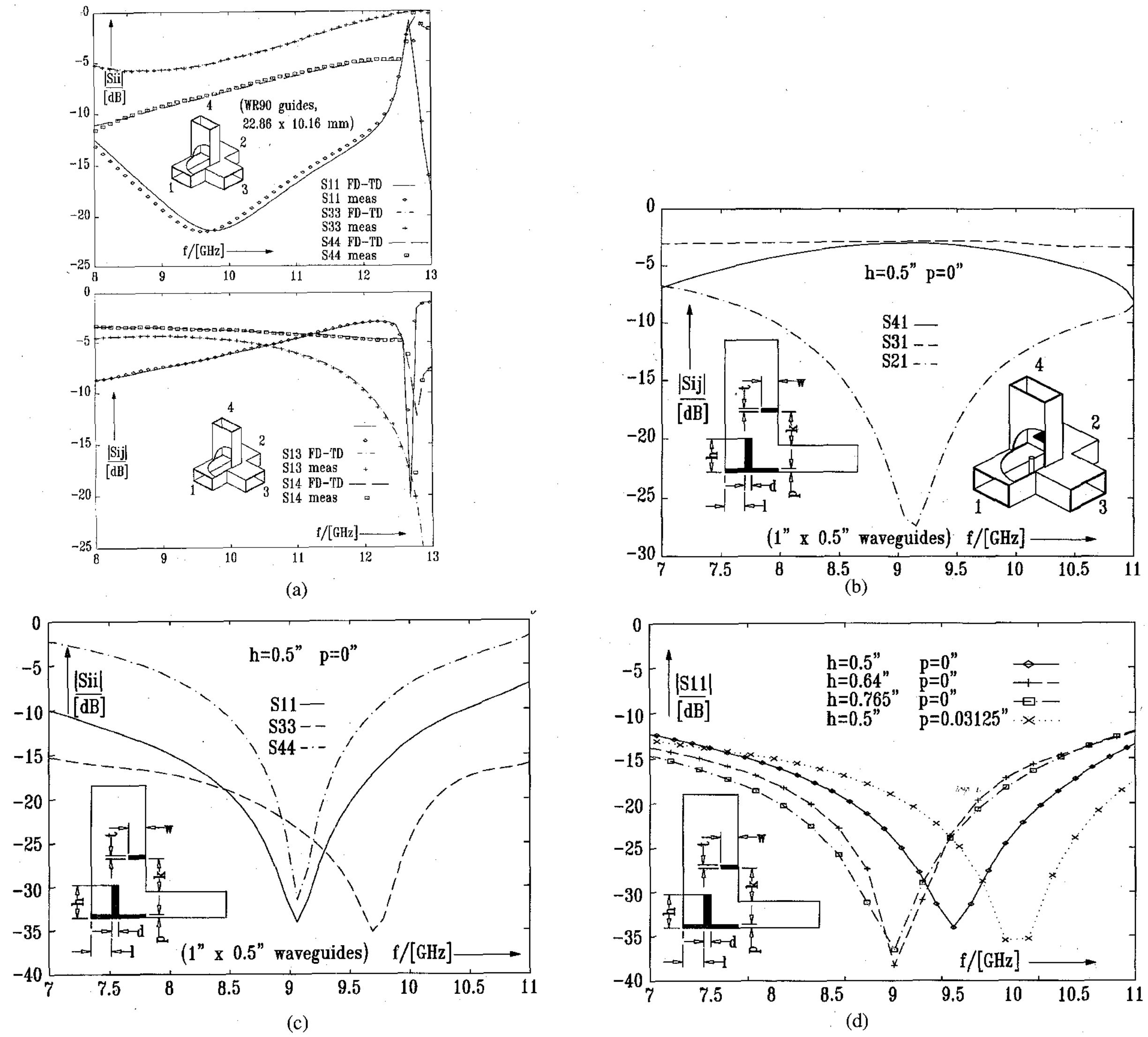

Fig. 5. Matched magic T. (a) Comparison theory (——), (- · · ·), (- - -) with measurements (◇+□) at the unmatched magic T. Dimensions: WR90 waveguides. Discretization: 97 920 cells in three grids. (b) Influence of additional matching elements, post and asymmetric iris, on the 3 dB and isolation behavior. (c) Influence on the return losses. (d) Influence of different post heights and of an additional plate. Dimensions: 1″× 0.5″waveguides. Discretization: 100 224 cells in three grids.

In the case of homogeneously filled waveguide ports, the eigenvectors $\vec{e}_{tq}^{\,j}$ and $\vec{h}_{tq}^{\,j}$ are frequency-independent, so that the modal extraction in (15) can be performed more efficiently in the time domain. The matrix-pencil method is then applied to obtain the poles and residues of the time signal. After that the frequency dependent modal amplitudes w_q^j are calculated from the poles as described earlier.

III. Results

In all investigated cases, the whole time interval for the FDTD simulation is chosen to be approximately four times the value which an exited wave needs to cross the structure under investigation. The first example is a twisted rectangular X-band waveguide in Fig. 2. Very good agreement with own finite element/mode-matching (FE/MM) calculations [27] is shown by using the described modal unmatched-port S-parameter technique. In contrast to the application of a 16 384-FFT, merely the first 1280 time iterations are required by using the matrix pencil technique, $N_{\text{skip}} = 1$ was used. A comparison of the matrix-pencil results with DFT-results, obtained with only 1280 time steps is shown in Fig. 2 also. It can be seen, that the S-parameters from the DFT are not yet convergent; it also should be mentioned that the knowledge of the poles and the residues of the signal enables the calculation of the frequency domain data at arbitrary frequency, this is an additional advantage over the discrete Fourier transform methods where the frequency is discrete with Δf which decreases with increasing total simulation time. For the standard matched-load S-parameter extraction technique (dot-dashed lines), only good agreement at the matched frequency (12 GHz) of the applied 1st-order ABC's may be stated. The same is true for the twisted 90°-bend, Fig. 3, the second example. Here, a value of three was used for N_{skip}. For the examples in Figs. 2 and 3, a nonorthogonal mesh has advantageously been chosen.

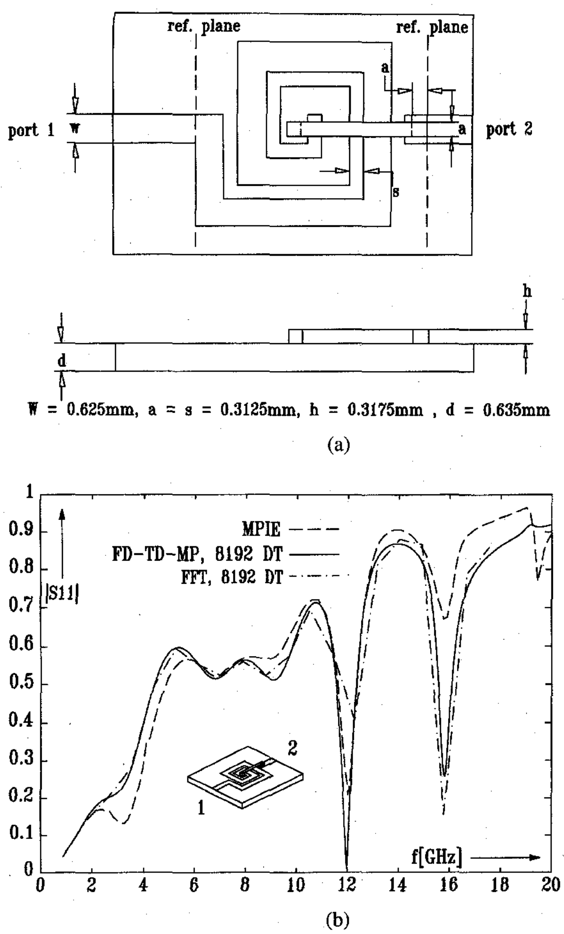

Fig. 6. Spiral inductor with an air bridge according to [30]. (a) Dimensions. (b) Verification of the FDTD/matrix-pencil results (——) with the MPIE-MoM results (- - -) and comparison to FFT results (- · -) after 8192 time steps (total FDTD-matrix-pencil time samples: 500, $N_{\mathrm{skip}} = 16$). Discretization: 28 × 100 × 169 cells.

The next example is a waffle-iron filter with the dimensions given in [28]. Good agreement with the FE/MM results may be stated again, Fig. 4(a). Also here, the standard matched load approach is only valid for exactly the matching frequency, cf. Fig. 4(b). Fig. 4(c) demonstrates that only 15 000 time steps ($N_{\mathrm{skip}} = 10$) are required for exact S-parameters as compared with the more than 65 000 time steps required by the traditional FFT.

A matched magic T for an X-band waveguide is chosen in Fig. 5. Fig. 5(a) demonstrates the excellent agreement between theory and measurements for the empty magic T. Additional matching elements, an asymmetric iris in port four and a circular post of partial height h, improve the 3 dB and the return loss behavior significantly, Fig. 5(b) and (c). The influence of the post height is demonstrated in Fig. 5(d) an additional plate provides an additional parameter for a frequency shift of the return loss curve.

In order to demonstrate the convenient applicability of the presented FDTD/matrix-pencil method also for the efficient calculation of scattering parameters of more complicated MMIC structures, a spiral inductor with an air bridge [30] is chosen (Fig. 6). Good agreement with the SDA results of [30] and with results obtained by a space-domain MPIE technique may be stated.

IV. Conclusion

A very efficient FDTD/matrix-pencil technique is presented for the analysis of waveguiding structures of nearly arbitrary shape. The method requires less numerical effort than, for instance, the often used combination with Prony's method. The application of the modal S-parameter definition for unmatched ports achieves even with standard Mur's absorbing boundaries excellent and reliable results also for the higher-order modes. A structure dependent mesh is used based on nonorthogonal or contour path grid cells, respectively, according to the specific form of the boundary. The proposed method is verified by excellent agreement with measurements, with FE/MM, or moment method results.

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