Numerical Solutions for the Simulation of Monolithic Microwave Integrated Circuits

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Abstract

The electric properties of monolithic microwave integrated circuits can be described in terms of their scattering matrix using Maxwellian equations. The corresponding three-dimensional boundary value problem of Maxwell's equations can be solved by means of a finite-volume scheme in the frequency domain. This results in a two-step procedure: a time and memory consuming eigenvalue problem for nonsymmetric matrices and the solution of a large-scale system of linear equations with indefinite symmetric matrices. Improved numerical solutions for these two linear algebraic problems are treated.

Contents

List of Figures

1 Introduction

The design of monolithic microwave integrated circuits (MMIC) requires efficient CAD tools in order to avoid costly and time-consuming redesign cycles. Commonly, network-oriented methods are used for this purpose. With increasing frequency and growing packaging density, however, the coupling effects become critical and the simple low-frequency models fail. Thus, field-oriented simulation methods become an indispensable tool for circuit design.

Figure 1 illustrates the principal structure under investigation. Since the electric properties are described in terms of the scattering matrix, transmission-line sections have to be attached at the ports. This defines propagation constants and mode patterns required for scattering matrix calculation. Typical line structures are planar lines (microstrip, coplanar waveguide), coaxial lines, or rectangular waveguides. The scattering matrix describes the struc-

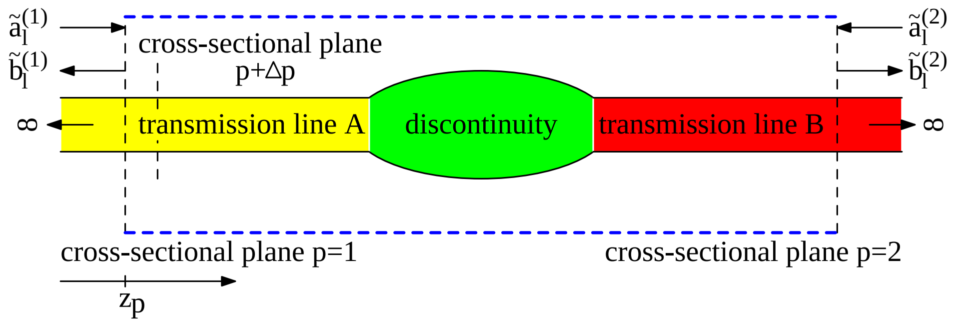

Figure 1: Structure under investigation

ture in terms of wave modes at the ports [2], [3], [1], [4], [5], which can be computed from the electromagnetic field. A three-dimensional boundary value problem can be formulated using Maxwell's equations in order to compute the electromagnetic field.

The application of the finite-volume method to the three-dimensional boundary value problem for the Maxwellian equations results in the so-called **F**inite-**D**ifference method in the **F**requency **D**omain (FDFD).

The program package F3D (Finite Differenzen dreidimensional) [3], [1] allows to simulate the electromagnetic field of nearly arbitrarily shaped structures.

2 Scattering Matrix

The transmission lines of the structure must be longitudinally homogeneous. The junction of the transmission lines, the so-called discontinuity, may have an arbitrary structure. A short part of the transmission lines is considered as a part of the discontinuity. The whole structure may be surrounded with an enclosure. Cross-sectional planes $p = 1$ and $p = 2$, so-called ports, are defined on the transmission lines. The incoming modes $\tilde{a}_l^{(p)}$ are changed in the discontinuity (see Figure 1). The complex generalized scattering matrix S describes the energy exchange and phase relation between all outgoing modes $\tilde{b}_l^{(p)}$ and all incoming modes $\tilde{a}_l^{(p)}$ [5].

$$S = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1m_{\overline{s}}} \\ S_{21} & S_{22} & \cdots & S_{2m_{\overline{s}}} \\ \cdots & \cdots & \cdots & \cdots \\ S_{m_{\overline{s}}1} & S_{m_{\overline{s}}2} & \cdots & S_{m_{\overline{s}}m_{\overline{s}}} \end{pmatrix} = (S_{\rho,\sigma}), \tag{1}$$

$$\rho, \sigma = 1(1)m_{\overline{s}}, \quad m_{\overline{s}} = \sum_{p=1}^{\overline{p}} m^{(p)}.$$

$m^{(p)}$ is the number of modes which have to be taken into account on the cross-sectional plane p. $\overline{p}$ is the number of cross-sectional planes.

The scattering matrix can be extracted from the orthogonal decomposition of the electric field at a pair of two neighboring cross-sectional planes p and $p + \Delta p$ (see Figure 1) on each waveguide for a number of linear independent excitations of the transmission lines. Therefore, we need the electric field. The electric field is computed using a boundary value problem for the Maxwellian equations.

3 The Boundary Value Problem

Because the scattering matrix is defined in the frequency domain, it is convenient to restrict oneself to fields which vary with the time t according to the complex exponential function $e^{\jmath\omega t}$. Thus, we use the integral form of the Maxwellian equations in the frequency domain:

$$\begin{aligned} \oint_{\partial\Omega} \frac{1}{\tilde{\mu}\mu_0} \vec{B} \cdot d\vec{s} &= \int_{\Omega} (\jmath\omega\tilde{\epsilon}\epsilon_0 \vec{E}) \cdot d\vec{\Omega}, \quad & \oint_{\cup\Omega} (\tilde{\epsilon}\epsilon_0 \vec{E}) \cdot d\vec{\Omega} &= 0, \\ \oint_{\partial\Omega} \vec{E} \cdot d\vec{s} &= \int_{\Omega} (-\jmath\omega\vec{B}) \cdot d\vec{\Omega}, \quad & \oint_{\cup\Omega} \vec{B} \cdot d\vec{\Omega} &= 0, \end{aligned} \tag{2}$$

taking into account the constitutive relations

$$\vec{B} = \mu\vec{H}, \quad \vec{D} = \epsilon\vec{E}, \quad \text{with} \quad \underline{\epsilon} = \epsilon + \frac{\kappa}{\jmath\omega}, \quad \mu = \tilde{\mu}\mu_0, \quad \underline{\epsilon} = \tilde{\epsilon}\epsilon_0.$$

The two equations on the right-hand side of (2) correspond to Gauss' flux laws. The field vectors $\vec{E}$, $\vec{H}$, $\vec{D}$, and $\vec{B}$ (electric and magnetic field intensity, electric and magnetic flux density, respectively) are complex functions of the spatial coordinates only. ω is the circular frequency and $\jmath^2 = -1$. The permeability μ, the permittivity ϵ, and the conductivity κ are assumed to be scalar functions of the spatial coordinates. $\underline{\epsilon}$ is the complex permittivity.

Boundary conditions

At the enclosure, except at the cross-sectional planes, the tangential electric or the tangential magnetic field is known. At the cross-sectional planes p the transverse electric field $\vec{E}_t^{(p)} = \vec{E}_t(z_p)$ is given by superposing transmission line modes $\vec{E}_{t,l}^{(p)} = \vec{E}_{t,l}(z_p)$ with weighted mode-amplitude sums $w_l^{(p)} = w_l(z_p)$. The transverse electric mode fields $\vec{E}_{t,l}^{(p)}$ are computed using an eigenvalue problem for transmission lines (see section 6).

The transverse mode fields $\vec{E}_{t,l}^{(p)}$ satisfy an orthogonality relation ($\delta_{l,m}$ Kronecker symbol).

$$\vec{E}_t^{(p)} = \sum_{l=1}^{m^{(p)}} w_l^{(p)} \vec{E}_{t,l}^{(p)}, \quad \int_\Omega (\vec{E}_{t,l}^{(p)} \times \vec{H}_{t,m}^{(p)}) \cdot d\vec{\Omega} = \eta_m \delta_{l,m}, \quad \eta_m = 1[W]. \tag{3}$$

This means that a three-dimensional boundary value problem of the Maxwellian equations is formulated.

The orthogonality relation is applied at two neighboring cross-sectional planes z_p and $z_{p+\Delta p} = z_p + \Delta z_p$ (see Figure 1):

$$\begin{aligned} \frac{1}{\eta_m}\int_\Omega (\vec{E}_t^{(p)} \times \vec{H}_{t,m}^{(p)}) \cdot d\vec{\Omega} &= \tilde{a}_m^{(p)} + \tilde{b}_m^{(p)} &&= w_m^{(p)}, \\ \frac{1}{\eta_m}\int_\Omega (\vec{E}_t^{(p+\Delta p)} \times \vec{H}_{t,m}^{(p)}) \cdot d\vec{\Omega} &= \tilde{a}_m^{(p+\Delta p)} + \tilde{b}_m^{(p+\Delta p)} &&= w_m^{(p+\Delta p)}. \end{aligned} \tag{4}$$

The weighted mode-amplitude sums $w_l^{(p)}$ are given. Because of

$$\tilde{a}_m^{(p+\Delta p)} = \tilde{a}_m^{(p)} e^{-\jmath k_{z_l}^{(p)} \Delta z_p}, \qquad \tilde{b}_m^{(p+\Delta p)} = \tilde{b}_m^{(p)} e^{+\jmath k_{z_l}^{(p)} \Delta z_p} \tag{5}$$

we can eliminate $\tilde{a}_m^{(p+\Delta p)}$ and $\tilde{b}_m^{(p+\Delta p)}$ from (4). Obtaining the mode amplitudes $\tilde{a}_m^{(p)}$ and $\tilde{b}_m^{(p)}$ we can compute the scattering matrix (1) [5].

4 The Maxwellian Grid Equations

It is advantageous to solve the Maxwellian equations directly rather than solving a partial differential equation of second order derived therefrom, because the quantities $\tilde{\mu}$ and $\tilde{\epsilon}$ can be different from cell to cell when using Maxwellian equations. The region is divided into elementary rectangular par-

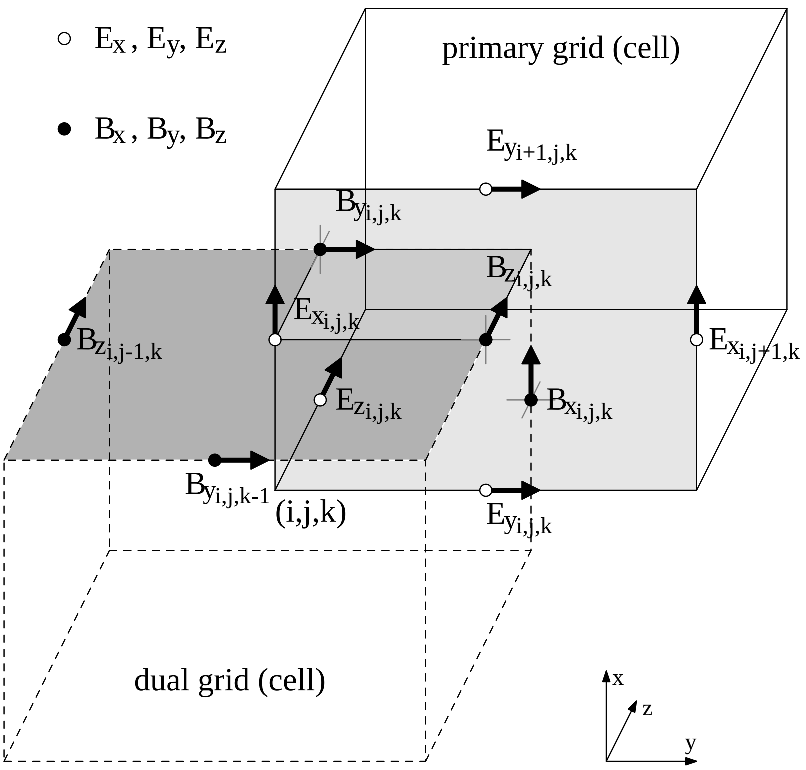

Figure 2: Primary and dual grid

allelepipeds by using a three-dimensional nonequidistant orthonormal Cartesian grid. The components E_x, E_y, and E_z of the electric field $\vec{E}$ are located in the centers of the edges of the elementary cells. The components B_x, B_y, and B_z, on the other hand are normal to the face centers [9], [8]. Thus, the electric field components form a primary grid and the magnetic flux density components a dual grid (see Figure 2). Using the lowest-order integration formulae

$$\oint_{\partial\Omega} \vec{f} \cdot d\vec{s} \approx \sum(\pm f_i s_i), \quad \int_{\Omega} \vec{f} \cdot d\vec{\Omega} \approx f\Omega \tag{6}$$

to approximate the integrals in (2) we get the matrix representation of Maxwell's equations:

$$\begin{aligned} A^T D_{s/\tilde{\mu}} \vec{b} &= \jmath\omega\epsilon_0\mu_0 D_{A\tilde{\epsilon}} \vec{e}, & B D_{A\tilde{\epsilon}} \vec{e} &= 0, \\ A D_s \vec{e} &= -\jmath\omega D_A \vec{b}, & B^T D_A \vec{b} &= 0 \end{aligned} \tag{7}$$

with

$$\vec{e} = \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix}, \quad \begin{aligned} \vec{e}_x &= (e_{x_1}, e_{x_2}, \ldots, e_{x_{n_{xyz}}})^T, \\ \vec{e}_y &= (e_{y_1}, e_{y_2}, \ldots, e_{y_{n_{xyz}}})^T, \\ \vec{e}_z &= (e_{z_1}, e_{z_2}, \ldots, e_{z_{n_{xyz}}})^T, \end{aligned} \quad \begin{aligned} e_{x_l} &= E_{x_{i,j,k}}, \\ e_{y_l} &= E_{y_{i,j,k}}, \\ e_{z_l} &= E_{z_{i,j,k}}, \end{aligned} \tag{8}$$

$$\vec{b} = \begin{pmatrix} \vec{b}_x \\ \vec{b}_y \\ \vec{b}_z \end{pmatrix}, \quad \begin{aligned} \vec{b}_x &= (b_{x_1}, b_{x_2}, \ldots, b_{x_{n_{xyz}}})^T, \\ \vec{b}_y &= (b_{y_1}, b_{y_2}, \ldots, b_{y_{n_{xyz}}})^T, \\ \vec{b}_z &= (b_{z_1}, b_{z_2}, \ldots, b_{z_{n_{xyz}}})^T, \end{aligned} \quad \begin{aligned} b_{x_l} &= B_{x_{i,j,k}}, \\ b_{y_l} &= B_{y_{i,j,k}}, \\ b_{z_l} &= B_{z_{i,j,k}}, \end{aligned} \tag{9}$$

$$\ell = (k-1)n_{xy} + (j-1)n_x + i, \quad n_{xy} = n_x n_y, \quad n_{xyz} = n_x n_y n_z.$$

The vectors $\vec{e}$ and $\vec{b}$ contain the components of the electric field and the components of the magnetic flux density of the elementary cells, respectively. The diagonal matrices D_s and D_A contain the information on material and on dimension for the structure and the corresponding mesh. A represents the curl operator in the second Maxwellian equation of (2) using the primary grid. B represents the surface integral of the divergence. A and B are sparse and contain the values 1, -1, and 0 only.

5 The System of Linear Algebraic Equations

The two equations of the left-hand side of (7) form a system of linear algebraic equations of the electromagnetic field in the absence of any boundary conditions. Eliminating the components of the magnetic flux density the number of unknowns in this two equations can be reduced by a factor of two:

$$Q_1\vec{e} = 0, \quad Q_1 = A^T D_{s/\tilde{\mu}} D_A^{-1} A D_s - k_0^2 D_{A\tilde{\epsilon}}, \quad k_0 = \omega\sqrt{\epsilon_0\mu_0}. \qquad (10)$$

Taking into account the boundary conditions we get a partitioning of the matrix Q_1 into a sum of two matrices

$$Q_1\vec{e} = (Q_{1,A} + Q_{1,r})\vec{e} = 0,$$

and we have to solve

$$\tilde{Q}_{1,A}\vec{\tilde{e}} = \vec{\tilde{r}}, \quad \tilde{Q}_{1,A} = D_s^{\frac{1}{2}} Q_{1,A} D_s^{-\frac{1}{2}}, \quad \vec{\tilde{r}} = D_s^{\frac{1}{2}}\vec{r}, \quad \vec{r} = -Q_{1,r}\vec{e}. \qquad (11)$$

Adding the matrix representation of the gradient of the electric-field divergence, which is equal to zero for fields without space charge,

$$\tilde{\epsilon}\epsilon_0\nabla(\frac{1}{(\tilde{\epsilon}\epsilon_0)^2}\nabla\cdot\tilde{\epsilon}\epsilon_0\vec{E}) = 0 \quad \Rightarrow \quad Q_2\vec{e} = 0$$

with

$$Q_2 = D_s^{-1} D_{A\tilde{\epsilon}} B^T D_{V\tilde{\epsilon}\tilde{\epsilon}}^{-1} B D_{A\tilde{\epsilon}}$$

to (11) gives the system

$$(\tilde{Q}_{1,A} + \tilde{Q}_{2,A})\vec{\tilde{e}} = \vec{\tilde{r}} \qquad (12)$$

with

$$\tilde{Q}_2 = D_s^{\frac{1}{2}} Q_2 D_s^{-\frac{1}{2}}, \quad \tilde{Q}_2 = \tilde{Q}_{2,A} + \tilde{Q}_{2,r}, \quad \vec{\tilde{e}} = D_s^{\frac{1}{2}}\vec{e}, \quad \tilde{Q}_{2,r}\vec{\tilde{e}} = 0, \quad \tilde{Q}_{2,A}\vec{\tilde{e}} = 0$$

which can be solved numerically faster [1]. The effect of this additional term can be interpreted as preconditioning. The system of linear algebraic equations is solved using multicoloring or independent set orderings to reduce the dimension of the system. The reduced systems are solved using iterative methods with preconditioning. The execution time was reduced by a factor of 10 in comparison to the original package F3D.

6 The Eigenvalue Problem

Before we can solve the system of linear equations we have to compute the transverse electric mode fields $\vec{E}_{t,l}^{(p)}$ at the port for the boundary condition using an eigenvalue problem. We consider a selected transmission line in the discussion to follow. $\tilde{\epsilon}$ and $\tilde{\mu}$ are functions of transverse position but are independent of the longitudinal direction. Thus, we assume that the fields vary exponentially in the longitudinal direction :

$$\vec{E}(x, y, z \pm 2h) = \vec{E}(x, y, z)e^{\mp \jmath k_z 2h}. \tag{13}$$

k_z is the propagation constant. A substitution of the ansatz (13) into the system of linear equations (10) taking into account boundary conditions, and the elimination of the longitudinal electric field components by means of the electric-field divergence equation (see 7)) gives an eigenvalue problem [4] for the transverse electric field on the transmission line region:

$$M(h^2)\underline{\vec{e}} = \gamma(h)\underline{\vec{e}} \ , \quad \mathrm{type}(M) = (2n_{xy} - n_b, 2n_{xy} - n_b). \tag{14}$$

The sparse matrix M is nonsymmetric. $\underline{\vec{e}}$ consists of components $E_{x_{i,j,k}}$ and $E_{y_{i,j,k}}$, $k = const$, of the eigenfunctions. The size of n_b depends on the boundary conditions at the port. The propagation constants k_z (16) can be computed from γ (15) after the solution of the eigenvalue problem (14):

$$\gamma_\iota(h) = e^{-\jmath k_{z_\iota} 2h} + e^{+\jmath k_{z_\iota} 2h} - 2 = -4\sin^2(k_{z_\iota} h) = u_\iota + \jmath v_\iota, \tag{15}$$

$$k_{z_\iota} = \frac{\jmath}{2h} \ln\left(\frac{\gamma_\iota}{2} + 1 + \sqrt{\frac{\gamma_\iota}{2}\left(\frac{\gamma_\iota}{2} + 2\right)}\right) = \beta_\iota - \jmath\alpha_\iota, \ \ \iota = 1(1)2n_{xy} - n_b. \tag{16}$$

The energy of the complex and evanescent modes decreases exponentially with the distance from the discontinuity. Thus, most of the modes can be neglected within the limit of accuracy. Generally speaking, the larger the magnitude of the imaginary part of k_z the stronger the decay. Therefore, the propagation constants k_{z_ι}, $\iota = 1(1)2n_{xy} - n_b$, are sorted in ascending order of $\mid \alpha_\iota \mid$. In the case if some $\mid \alpha_\iota \mid$ have the same value the constants k_{z_ι} are sorted in descending order of $\mid \beta_\iota \mid$.

In the original version of the program package F3D all propagation constants are computed and sorted in order to select the wanted propagation constants. This way is very time-consuming. The full matrix is stored.

In order to avoid the time-consuming computation of all eigenvalues γ we use the implicitly restarted Arnoldi iteration [7], [6] now, which is carried out twice to find the first propagation constants of the sorted set.

Using the iterative method the computation of the needed propagation constants in a typical example is 40-fold faster than in the old version. The reduction of the memory consumption amounts the 20-fold, since the sparse storage technique is applied.

7 Conclusions

The Finite Difference method in Frequency Domain allows the calculation of the scattering matrix for a number of simultaneously excited modes. This is an advantage compared with computations in the Time Domain. The price to be paid is the high memory consumption and the time-consuming solution of an eigenmode problem of high dimension and of large systems of linear algebraic equations.

We avoid the time-consuming computation of all eigenvalues in order to calculate a selected set of propagation constants using an iterative method that is carried out twice. We find that the SSOR preconditioning combined with the multicoloring or independent set orderings is a very efficient method to solve the systems of linear equations. The numerical effort and the storage requirements can be reduced considerably.

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