Improved Numerical Solutions for the Simulation of Microwave Circuits

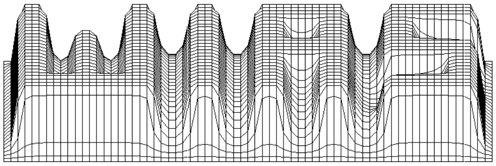
Georg Hebermehl*
Rainer Schlundt †

*Weierstrass Institute for Applied Analysis and Stochastics,
Mohrenstr. 39, D-10117 Berlin, Germany*

Horst Zscheile‡
Wolfgang Heinrich §

*Ferdinand-Braun-Institut für Höchstfrequenztechnik,
Rudower Chaussee 5, D-12489 Berlin, Germany*

January 16, 1997



1991 Mathematics Subject Classification. 35Q60, 35L20, 65F10, 65F50, 65N22.
Keywords. Maxwell's equations, finite-difference method, system of simultaneous linear equations, independent set orderings, SSOR preconditioner.

*e-mail: hebermehl@wias-berlin.de, URL: http://hyperg.wias-berlin.de
†e-mail: schlundt@wias-berlin.de, URL: http://hyperg.wias-berlin.de
‡e-mail: zscheile@fbh-berlin.de, URL: http://www.fta-berlin.de
§e-mail: heinrich@fbh-berlin.de, URL: http://www.fta-berlin.de

Abstract

The electromagnetic characteristics of microwave circuits can be described by the scattering matrix. This results in a three-dimensional boundary value problem, which can be solved using the Finite Difference method in the Frequency Domain (FDFD). A time consuming part of the FDFD-method is the solution of large systems of linear algebraic equations. The coefficient matrix is sparse, symmetric, and indefinite. Using multicoloring and independent set orderings essential numerical improvements are achieved.

Contents

List of Figures

1 Introduction

Maxwell's equations in a general source-free and linear medium in a time-harmonic and integral form can be expressed as

$$\nabla \times \vec{\mathcal{H}} = \frac{\partial \vec{\mathcal{D}}}{\partial t} \quad \Rightarrow \quad \oint_{\partial\Omega} \frac{1}{\mu_r \mu_0} \vec{B} \cdot d\vec{s} = \int_{\Omega} (\jmath\omega\epsilon_r\epsilon_0 \vec{E}) \cdot d\vec{\Omega} \qquad (1)$$

$$\nabla \times \vec{\mathcal{E}} = -\frac{\partial \vec{\mathcal{B}}}{\partial t} \quad \Rightarrow \quad \oint_{\partial\Omega} \vec{E} \cdot d\vec{s} = \int_{\Omega} (-\jmath\omega \vec{B}) \cdot d\vec{\Omega} \qquad (2)$$

$$\nabla \cdot \vec{\mathcal{D}} = 0 \;\; \Rightarrow \;\; \oint_{\cup\Omega} (\epsilon_r \epsilon_0 \vec{E}) \cdot d\vec{\Omega} = 0 \tag{3}$$

$$\nabla \cdot \vec{\mathcal{B}} = 0 \;\; \Rightarrow \;\; \oint_{\cup\Omega} \vec{B} \cdot d\vec{\Omega} = 0 \;\; , \tag{4}$$

where $\vec{\mathcal{E}}(\vec{r},t) = \vec{E}(\vec{r})e^{\jmath\omega t}$ and $\vec{\mathcal{H}}(\vec{r},t) = \vec{H}(\vec{r})e^{\jmath\omega t}$ are the electric and magnetic field intensity vectors, respectively, $\vec{\mathcal{D}}(\vec{r},t) = \vec{D}(\vec{r})e^{\jmath\omega t}$ and $\vec{\mathcal{B}}(\vec{r},t) = \vec{B}(\vec{r})e^{\jmath\omega t}$ are the electric and magnetic flux density vectors, respectively, $\mu(\vec{r}) = \mu_r(\vec{r})\mu_0$ and $\epsilon(\vec{r}) = \epsilon_r(\vec{r})\epsilon_0$ are the permeability and permittivity, respectively, and ω is the angular frequency of the sinusoidal excitation. The time dependence is $e^{\jmath\omega t}$, which is not printed.

Constitutive relations between the field quantities are determined by the macroscopic properties of the medium being considered.

$$\vec{D} = \epsilon \vec{E} \tag{5}$$

$$\vec{B} = \mu \vec{H} \tag{6}$$

We wish to solve Maxwell's equations on a regular three-dimensional domain $\mathcal{V}$ that has a closed boundary surface denoted by $\partial\mathcal{V}$. We assume that the domain $\mathcal{V}$ has been discretized into structured orthogonal hexahedral cells. Each cell has a closed boundary surface denoted by $\cup\Omega$. Each face Ω is surrounded by a closed contour $\partial\Omega$. The linear isotropic material properties ϵ_r and μ_r are constant in each cell. In this paper, only lossless materials are taken into consideration. Therefore, the quantities ϵ_r and μ_r are real. The boundary conditions on $\partial\mathcal{V}$ are as follows: On some parts of the surface the tangential electric field is given by an eigenvalue problem (see [2] and [6]). These parts of $\partial\mathcal{V}$ are called ports. On the remaining parts of $\partial\mathcal{V}$ either the tangential electric field $\vec{E}_{tan}$ or the tangential magnetic field $\vec{H}_{tan}$ vanishes. In the former case the surface is called electric wall, and it describes a metal with infinite conductivity. The case $\vec{H}_{tan} = 0$ is called magnetic wall. This concept is useful to describe a symmetry plane of the field (which allows to reduce the domain $\mathcal{V}$ to one half of the volume of the structure under investigation).

The elementary cell of the Yee grid [13] is shown in Figure 1. The locations of the electric and magnetic fields do not coincide with the nodes {i,j,k} of the Cartesian grid. The electric field components are located at the centers of the edges of the cell and the magnetic flux density components are normal to the centers of the faces. The FDFD-method requires the use of a dual grid.

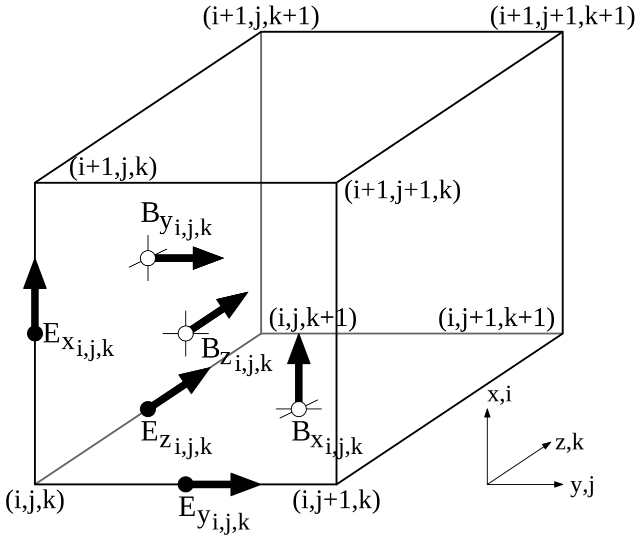


Figure 1: The elementary cell for the Yee algorithm with sampling locations of field quantities.

The dual grid and its structure are completely derivable from a knowledge of the primary grid. Figure 2 shows an eight cell hexahedral primary grid and its one interior dual cell. The primary grid is the grid that is initially created. The electric field components lie on the centers of the edges of the primary cell. We define the barycenters of all primary cells. Then we construct edges of the dual grid (dual edges) by connecting barycenters of adjacent cells with straight lines. The barycenters of two cells will be connected if and only if the two cells have a common face. Then the magnetic flux density components lie on the dual edges, i.e. on the edges of the dual cell.

2 The System of Algebraic Equations

We use the lowest-order integration formulae

$$\oint_{\partial\Omega} \vec{f} \cdot d\vec{s} \approx \sum_i f_i * (\pm s_i) \quad , \quad \int_\Omega \vec{f} \cdot d\vec{\Omega} \approx f\Omega \tag{7}$$

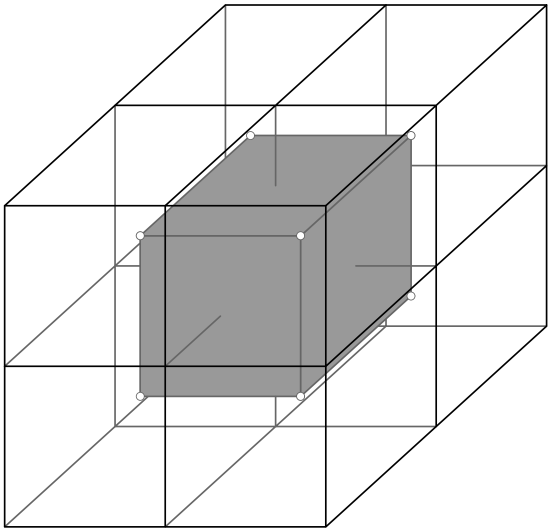


Figure 2: An eight cell primary grid and its one interior dual cell.

in order to approximate Maxwell's equations (see (1 - 4)). The closed path $\partial\Omega$ of the integration consists of straight lines of length s_i and is the path around the periphery of any cell face Ω of the primary and dual grid, respectively. The algebraic sign of length s_i in (7) depends on the direction of integration. f_i denotes the function value on the line with the length s_i. Ω is the area of any cell face of the primary and dual grid, respectively. The function value f lies on the cell face Ω.
Let be

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

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

with

$$l = (k-1)n_{xy} + (j-1)n_x + i \ , \ n_{xy} = n_x n_y \ , \ n_{xyz} = n_x n_y n_z \quad , \tag{10}$$

and

$$i = 1, \ldots, n_x, \quad j = 1, \ldots, n_y \quad \text{and} \quad k = 1, \ldots, n_z \tag{11}$$

the vectors containing the electric field and magnetic flux density of the elementary cells, respectively. The value n_s, $s \in \{x, y, z\}$, denotes the number of elementary cells in the s-direction.
Applying (7) to Equ. (2) yields (see [12])

$$\oint_{\partial\Omega} \vec{E} \cdot d\vec{s} = \int_{\Omega} (-\jmath\omega\vec{B}) \cdot d\vec{\Omega} \quad \Rightarrow \quad AD_s\vec{e} = -\jmath\omega D_A\vec{b} \ . \tag{12}$$

The matrix A represents the curl operator in the Maxwellian equation (2) and consists only of the elements -1, 0 and 1. The diagonal matrices D_s and D_A contain the information on cell dimensions for the specified structure.
Similarly, one has for Equ. (1)

$$\oint_{\partial\Omega} \frac{1}{\mu_r\mu_0}\vec{B} \cdot d\vec{s} = \int_{\Omega} (\jmath\omega\epsilon_r\epsilon_0\vec{E}) \cdot d\vec{\Omega} \quad \Rightarrow \quad A^T D_{s/\mu}\vec{b} = \jmath\omega\epsilon_0\mu_0 D_{A\epsilon}\vec{e} \ . \tag{13}$$

Here, the matrix A^T represents the curl operator in the Maxwellian equation (1) and is the transposed matrix of A. The diagonal matrices $D_{s/\mu}$ and $D_{A\epsilon}$ contain the information on cell dimensions and material for the specified structure and the mesh.
Note that, strictly speaking, this approach represents a finite integration scheme. Nevertheless, since the resulting formulae are identical to the finite-difference form, in most cases the more common term FDFD is used.
We combine the Equations (12) and (13) to Equation (14) by substituting the magnetic flux density components:

$$Q_1\vec{e} = 0 \quad , \quad Q_1 = A^T D_{s/\mu} D_A^{-1} A D_s - k_0^2 D_{A\epsilon} \ , \tag{14}$$

where

$$k_0 = \omega\sqrt{\epsilon_0\mu_0} \ . \tag{15}$$

In order to determine the scattering matrix, ports are defined on the surface of the structure. There in- and outgoing wave modes act as sources for the field inside the domain (see [2] and [6]). Thus, a source term has to be induced by partitioning of the matrix Q_1:

$$Q_1 = Q_{1,A} + Q_{1,r} \quad \Rightarrow \quad Q_{1,A}\vec{e} = -Q_{1,r}\vec{e} \ , \tag{16}$$

where $Q_{1,r}\vec{e}$ is known. Using $\vec{r} = -Q_{1,r}\vec{e}$ the matrix $Q_{1,A}$ is transformed into a symmetric one, after some mathematical manipulations:

$$\tilde{Q}_{1,A}\vec{\tilde{e}} = \underbrace{D_s^{\frac{1}{2}} Q_1 D_s^{-\frac{1}{2}}}_{\tilde{Q}_{1,A}} \underbrace{D_s^{\frac{1}{2}}\vec{e}}_{\vec{\tilde{e}}} = -D_s^{\frac{1}{2}} Q_{1,r}\vec{e} = D_s^{\frac{1}{2}}\vec{r} = \vec{\tilde{r}} \ . \tag{17}$$

The matrix representation of the Maxwellian equation (3) for the dual grid reads:

$$\oint_{\cup\Omega} (\epsilon_r\epsilon_0\vec{E}) \cdot d\vec{\Omega} = 0 \quad \Rightarrow \quad BD_{A\epsilon}\vec{e} = 0 \ . \tag{18}$$

The matrix B represents the integral over a closed surface $\cup\Omega$ of the corresponding elementary cell and consists only of the elements -1, 0 and 1. We want to combine the information of Equations (17) and (18). Whereas (17) describes in the physical three-dimensional space a vectorial field, Equ. (18) represents a scalar one. Therefore, we build instead of (18) without loss of generality the vector equation

$$\epsilon_r\epsilon_0\nabla(\frac{1}{(\epsilon_r\epsilon_0)^2}\nabla \cdot \epsilon_r\epsilon_0\vec{E}) = 0 \ , \tag{19}$$

which is equivalent to the matrix equation (see [2], [6], [7] and [11])

$$Q_2\vec{e} = 0 \quad , \quad Q_2 = D_s^{-1}D_{A\epsilon}B^T D_{V\epsilon\epsilon}^{-1}BD_{A\epsilon} \ . \tag{20}$$

The diagonal matrix $D_{V\epsilon\epsilon}$ contains the information on cell dimensions and material.
We carry out a similar partitioning like (16) for the Equation (20) and then transform this equation into a symmetric one.
Using $Q_{2,r}\vec{e} = 0$ we get from (20):

$$Q_2 = Q_{2,A} + Q_{2,r} \quad \Rightarrow \quad \tilde{Q}_{2,A}\vec{\tilde{e}} = \underbrace{D_s^{\frac{1}{2}} Q_{2,A} D_s^{-\frac{1}{2}}}_{\tilde{Q}_{2,A}} \underbrace{D_s^{\frac{1}{2}}\vec{e}}_{\vec{\tilde{e}}} = -D_s^{\frac{1}{2}} \underbrace{Q_{2,r}\vec{e}}_{=0} = 0 \ . \tag{21}$$

3 The Numerical Solution of the System of Linear Algebraic Equations

Let be:

$A(n,n)$ matrix containing the entries of Maxwell's equations (1) and (2) (see (17), $A = \tilde{Q}_{1,A}$),

$B(n,n)$ matrix containing the entries of Maxwell's equation (3) (see (21), $B = \tilde{Q}_{2,A}$),

$M(n,n)$ preconditioner for the coefficient matrix A,

$x(n)$ vector containing the electric field components of all elementary cells (see (17), $x \equiv \tilde{\vec{e}} = D_s^{\frac{1}{2}} \vec{e}$),

$b(n)$ right-hand side (see (17), $b \equiv \tilde{\vec{r}} = D_s^{\frac{1}{2}} \vec{r}\,,\;\; \vec{r} = -Q_{1,r}\vec{e}$),

n number of equations (see (10) and (11), $n = 3n_{xyz}$).

We consider the solution of the non-singular system of n linear algebraic equations

$$Ax = b \ . \tag{22}$$

The matrix A is symmetric, indefinite and sparse with positive diagonal elements.

The sparse storage scheme used is a row-wise representation of the nonzero entries in the coefficient matrix of the linear system (22). For a nonsymmetric coefficient matrix, all of the nonzero values in each row are stored in a contiguous block of data. If the matrix is symmetric, computer memory can be saved by storing only the nonzero entries in each row on and above the main diagonal (see [9]). The data structure consists of three arrays:

- A real array A containing the real values a_{ij} stored row by row, from row 1 to n and in each row on and above the main diagonal, i.e., $i = 1, \cdots, n$ and $j \geq i$. The length of A is nnz.

- An integer array JA containing the column indices of the elements a_{ij} as stored in the array A. The length of JA is nnz.

- An integer array IA containing the pointers to the beginning of each row in the arrays A and JA. The length of IA is $n+1$ with $IA(n+1)$ containing the number $nnz+1$.

The complexity of iterative methods for solving linear systems (22) is $\mathcal{O}(n^2)$, whilst direct methods like LU and Cholesky decompositions are $\mathcal{O}(n^3)$. The convergence rate of iterative methods depends on spectral properties of the coefficient matrix A of (22). Hence one may attempt to transform the linear system (22) into one that is equivalent in the sense that it has the same solution but more favorable spectral properties. A preconditioner is a matrix that performs such a transformation. For instance, if a matrix M approximates the coefficient matrix A (22) in some way, the transformed system

$$M^{-1}Ax = M^{-1}b \tag{23}$$

has the same solution as the original system (22), but the spectral properties of its coefficient matrix $M^{-1}A$ may be more favorable. The above transformation of the linear system (22) to (23) is not what is used in practice. A more correct way of introducing the preconditioner would be to split the preconditioner as $M = M_1 M_2$ and to transform the system as

$$M_1^{-1}AM_2^{-1}(M_2x) = M_1^{-1}b \ . \tag{24}$$

The matrices M_1 and M_2 are called the left- and right-hand preconditioners, respectively (see [1]).
Using the linear system $Bx = 0$ ($B = \tilde{Q}_{2,A}$, see Eqn. (21)) we construct a preconditioner M for the original system (22):

$$M^{-1} = I + BA^{-1} \quad , \quad M = (I + BA^{-1})^{-1} \ . \tag{25}$$

Equations (23) and (25) can be combined to the system of linear equations (26) by substituting the matrix M^{-1}:

$$(I + BA^{-1})Ax = (I + BA^{-1})b \quad \Rightarrow \quad (A + B)x = b \quad \Rightarrow \quad \tilde{A}\tilde{x} = \tilde{b} \ , \tag{26}$$

where $\tilde{A} = A + B$, $\tilde{x} \equiv x$ and $\tilde{b} \equiv b$.
Compared with matrix (22), the eigenvalues of the system matrix (26) have shifted in the direction of the positive half plane [11].
A commonly used approach for solving large sparse linear systems is to resort to the general multicolor and independent set orderings. The goal of multicoloring is to determine a coloring of the nodes of the adjacency graph of a matrix in such a way that any two adjacency nodes do not have a common color. A basic algorithm for obtaining a multicoloring of an arbitrary graph is the following idea (see [10]):

1. Initially assign color number zero (uncolored) to every node.

2. Traverse the graph in any fashion.

3. Scan all nodes in the chosen order and at every node assign the smallest color number allowable, i.e.,

   $$color(i) = \min\{k > 0 \,|\, k \neq color(j), \forall j \in adj(i)\} \ ,$$

   where $adj(i)$ represents the set of nodes that are adjacent to node i.

Once the multicolor ordering is applied to the matrix, we obtain a block diagonal matrix whose diagonal blocks are diagonal matrices, e.g. for three colors

$$\begin{pmatrix} \boxed{D_1} & & F \\ & \boxed{D_2} & \\ E & & \boxed{D_3} \end{pmatrix} ,$$

where the D_i's are diagonal and E, F are general sparse matrices.
On the other hand one can dynamically find sets of unknowns which are independent. These unknowns are not coupled by the matrix. A set of such unknowns is called an independent set. Independent set orderings are permutations to transform the original matrix (26) in the form

$$\tilde{A} \quad \Rightarrow \quad \begin{pmatrix} \tilde{D} & \tilde{F} \\ \tilde{E} & \tilde{H} \end{pmatrix} , \tag{27}$$

where $\tilde{D}$ is a diagonal matrix, $\tilde{E}$ and $\tilde{F}$ are general sparse matrices and $\tilde{H}$ is a quadratic sparse matrix. If $\tilde{A}$ is a symmetric matrix, then $\tilde{F} = \tilde{E}^T$. We reduce the system (26) by eliminating the independent set $\tilde{D}$, and then obtain a smaller linear system which is again sparse. Then we can find an independent set for this reduced system. The process can be continued recursively a few times. One of the advantages of this approach is the fact that the reduced systems are usually much smaller than the original system. The drawback is that the reduced systems gradually lose their sparsity. Let $\tilde{A}_i$ be the matrix obtained at the i-th step of reduction for $i = 0, \ldots, n_{lev} - 1$ with $\tilde{A}_0 = \tilde{A}$ (see (26)). We apply an independent set ordering (see (27)) to $\tilde{A}_i$ to obtain a permuted matrix

$$\tilde{P}_i \tilde{A}_i \tilde{P}_i^T = \begin{pmatrix} \tilde{D}_i & \tilde{E}_i^T \\ \tilde{E}_i & \tilde{H}_i \end{pmatrix} . \tag{28}$$

The unknowns of the independent set $\tilde{D}_i$ are eliminated to get the next reduced matrix

$$\tilde{A}_{i+1} = \tilde{H}_i - \tilde{E}_i \tilde{D}_i^{-1} \tilde{E}_i^T \ . \tag{29}$$

Thus we have a sequence of block LU factorizations

$$\tilde{P}_i \tilde{A}_i \tilde{P}_i^T = \begin{pmatrix} \tilde{D}_i & \tilde{E}_i^T \\ \tilde{E}_i & \tilde{H}_i \end{pmatrix} = \begin{pmatrix} I & 0 \\ \tilde{E}_i \tilde{D}_i^{-1} & I \end{pmatrix} \cdot \begin{pmatrix} \tilde{D}_i & \tilde{E}_i^T \\ 0 & \tilde{A}_{i+1} \end{pmatrix} \tag{30}$$

with $\tilde{A}_{i+1}$ defined by (29).
Using independent set ordering (see (28)) we get a system of linear equations

$$\tilde{P}_i \tilde{A}_i \tilde{P}_i^T \tilde{y}_i = \tilde{c}_i \tag{31}$$

with $\tilde{y}_i = \tilde{P}_i \tilde{x}_i = (\tilde{y}_{i,1}, \tilde{y}_{i,2})^T$ and $\tilde{c}_i = \tilde{P}_i \tilde{b}_i = (\tilde{c}_{i,1}, \tilde{c}_{i,2})^T$. Thus we have to solve the system of linear equations

$$\underbrace{(\tilde{H}_i - \tilde{E}_i \tilde{D}_i^{-1} \tilde{E}_i^T)}_{\tilde{A}_{i+1}} \underbrace{\tilde{y}_{i,2}}_{\tilde{x}_{i+1}} = \underbrace{\tilde{c}_{i,2} - \tilde{E}_i \tilde{D}_i^{-1} \tilde{c}_{i,1}}_{\tilde{b}_{i+1}} \tag{32}$$

for $\tilde{y}_{i,2}$ $(\equiv \tilde{x}_{i+1})$ and

$$\tilde{y}_{i,1} = \tilde{D}_i^{-1} (\tilde{c}_{i,1} - \tilde{E}_i^T \tilde{x}_{i+1}) \tag{33}$$

for $\tilde{y}_{i,1}$. Then we have to permute the solution vector $\tilde{y}_i$ (32, 33) back to the vector $\tilde{x}_i$ (26).
We have to solve the last reduced system (see (32), $i = n_{lev} - 1$)

$$\tilde{A}_{n_{lev}} \tilde{x}_{n_{lev}} = \tilde{b}_{n_{lev}}$$

for $\tilde{x}_{n_{lev}}$. Let $\tilde{D}_{\tilde{A}_{n_{lev}}} = diag(\tilde{A}_{n_{lev}})$ the diagonal matrix of $\tilde{A}_{n_{lev}}$, then we set $\tilde{M}_1 = \tilde{M}_2 = \tilde{D}^{\frac{1}{2}}_{\tilde{A}_{n_{lev}}}$ and apply the preconditioning (24):

$$\tilde{A}_{n_{lev}} \tilde{x}_{n_{lev}} = \tilde{b}_{n_{lev}} \quad \Rightarrow \quad \underbrace{\tilde{D}^{-\frac{1}{2}}_{\tilde{A}_{n_{lev}}} \tilde{A}_{n_{lev}} \tilde{D}^{-\frac{1}{2}}_{\tilde{A}_{n_{lev}}}}_{\hat{A}} \underbrace{\tilde{D}^{\frac{1}{2}}_{\tilde{A}_{n_{lev}}} \tilde{x}_{n_{lev}}}_{\hat{x}} = \underbrace{\tilde{D}^{-\frac{1}{2}}_{\tilde{A}_{n_{lev}}} \tilde{b}_{n_{lev}}}_{\hat{b}} \ . \tag{34}$$

We construct a SSOR preconditioner (see [1]) for the matrix $\hat{A}$. If the matrix is decomposed as

$$\hat{A} = L + I + L^T \tag{35}$$

in its strictly lower triangular, diagonal, and strictly upper triangular part, the SSOR matrices, parametrized by ω are defined as

$$\hat{M}_1 = (I + \omega L) \quad , \quad \hat{M}_2 = (I + \omega L^T) \tag{36}$$

with $0 < \omega < 2$. The optimal value of the ω parameter will reduce the number of iterations to a lower order.
The matrix vector products with the coefficient matrix $\hat{A}$ (34, 35) of the preconditioned system (24, 36) can be computed very efficiently by using Eisenstat's trick (see [4]) when a SSOR preconditioner is used. We now show how the matrix vector product $(\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1})v$, for any vector v, can be computed efficiently.

$$\begin{aligned} \hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1} &= (I + \omega L)^{-1}(L + I + L^T)(I + \omega L^T)^{-1} \\ &= \tfrac{1}{\omega}((I + \omega L^T)^{-1} + (I + \omega L)^{-1}(I - (2 - \omega)(I + \omega L^T)^{-1})) \end{aligned}$$

The result $r = (\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1})v$ of the matrix vector product can be obtained as follows.

1. Solve $(I + \omega L^T)t = v$ for t.
2. Set $\tilde{t} = v - (2 - \omega)t$.
3. Solve $(I + \omega L)\hat{t} = \tilde{t}$ for $\hat{t}$.
4. Set $r = \frac{1}{\omega}(t + \hat{t})$.

Note that the above algorithm requires two solves with the triangular matrices $(I + \omega L)$ and $(I + \omega L^T)$ plus a few arithmetical operations.
We have solved the preconditioned system (24, 36) with the coefficient matrix $\hat{A}$ (34, 35) with conjugate gradient-like iterative methods described in [3], [5], [8].

4 Numerical Example

The reduction of the computing time is demonstrated by calculating of the scattering matrix of a structure consisting of a microstrip line on a dielectric substrate grounded at one end by a via hole. The structure is divided into $n_{xyz} = 60\,984$ elementary cells with $n_x = 33$, $n_y = 28$, and $n_z = 66$. The order of the system of linear algebraic equations is $n = 3n_{xyz} = 182\,952$.

The total number of nonzeros of the matrix $\tilde{A}$ $(= \tilde{A}_0)$ (26, 29) amounts to 1 145 738 for this example where only $nnz = 664\,345$ elements are stored. We apply an independent set ordering to the matrix $\tilde{A}_0$ with the level $n_{lev} = 1$ to obtain the reduced matrix $\tilde{A}_1$ (29). The order of the reduced system of linear equations (32) is $n_r = 84\,207$. The total number of nonzeros of the matrix $\tilde{A}_1$ amounts to 1 514 129. The number of stored nonzeros is $nnz_r = 799\,168$. We now consider four possibilities of preconditioning for the given coefficient matrix $\tilde{A}$ to solve the linear system of equations (26).

1. The Eqn. (34) is to be solved for $n_{lev} = 0$.

$$\tilde{D}_{\tilde{A}}^{-\frac{1}{2}} \tilde{A} \tilde{D}_{\tilde{A}}^{-\frac{1}{2}} \tilde{D}_{\tilde{A}}^{\frac{1}{2}} \tilde{x} = \tilde{D}_{\tilde{A}}^{-\frac{1}{2}} \tilde{b}$$

   This system of linear algebraic equations is used in [2].

2. Using the preconditioner $\hat{M} = \hat{M}_1 \hat{M}_2$ (see (36)) the system (34) is to be solved for $n_{lev} = 0$.

$$\hat{M}^{-1} \hat{A} \hat{x} = \hat{M}^{-1} \hat{b}$$

3. Using the preconditioner $\hat{M} = \hat{M}_1 \hat{M}_2$ (see (36)) the system (34) is to be solved for $n_{lev} = 1$.

$$\hat{M}^{-1} \hat{A} \hat{x} = \hat{M}^{-1} \hat{b}$$

4. The preconditioned system (24, 36) with the coefficient matrix $\hat{A}$ (34, 35) is to be solved for $n_{lev} = 1$ by using Eisenstat's trick.

$$\hat{M}_1^{-1} \hat{A} \hat{M}_2^{-1} (\hat{M}_2 \hat{x}) = \hat{M}_1^{-1} \hat{b}$$

Figure 3 shows the number of iterations and execution times (in seconds) for the four methods of preconditioning. The time data refer to a SGI workstation (Indy). The system of linear algebraic equations were solved by the algorithm described in [3]. The stopping criterion was in each case a reduction of the norm of the residual by 10^{-8}. Both the time for the iteration algorithm and the total time for the subroutine call are given. We observe that the SSOR preconditioner combined with the independent set ordering is very effective in solving the linear system of equations. Furthermore, Eisenstat's trick reduces the execution time.

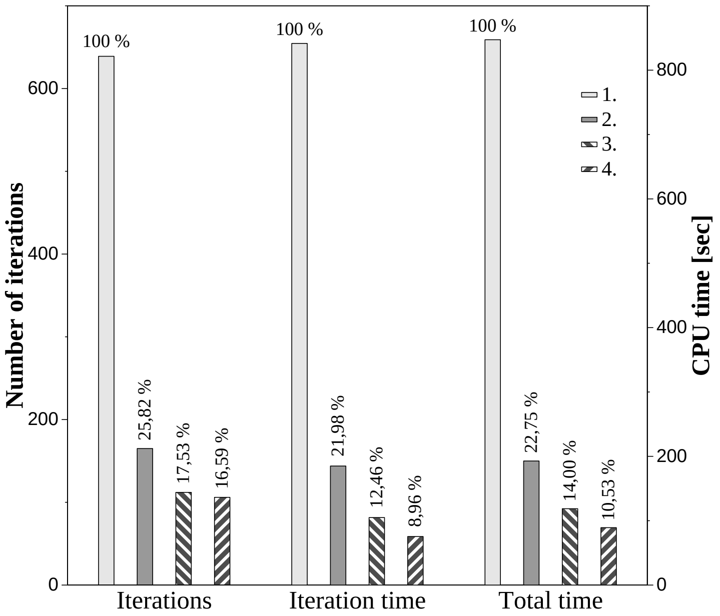


Figure 3: Number of iterations and execution times for the calculation of the scattering matrix.

5 Conclusions

The Finite Difference method in Frequency Domain allows the computation of the scattering matrix of a given structure for a number of simultaneously excited modes. This is an advantage compared with calculations in the Time Domain. The price to be paid is the time-consuming solution of large systems of linear algebraic equations. We have studied various methods to do this effectively and found that the SSOR preconditioning combined with the independent set ordering is a very efficient method. The Eisenstat trick can be used to compute a matrix-vector product with the preconditioned matrix $\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1}$ at a cost only slightly more than the cost of a matrix-vector product with $\hat{A}$.

References

[1] Barrett, R., Berry, M., Chan, T., Demmel, J., Donato, J., Dongarra, J., Eijkhout, V., Pozo, R., Romine, C., van der Vorst, H., *Templates for*

the Solution of Linear Systems: Building Blocks for Iterative Methods, SIAM, Philadelphia, PA, 1994.

[2] Beilenhoff, K., Heinrich, W., Hartnagel, H. L., *Improved Finite-Difference Formulation in Frequency Domain for Three-Dimensional Scattering Problems*, IEEE Transactions on Microwave Theory and Techniques, Vol. 40, No. 3, March 1992.

[3] Deuflhard, P., *A Study of Lanczos-Type Iterations for Symmetric Indefinite Linear Systems*, Preprint SC 93-6, Konrad-Zuse-Zentrum für Informationstechnik Berlin, March 1993.

[4] Eisenstat, S. C., *Efficient implementation of a class of preconditioned conjugate gradient methods*, SIAM J. Sci. Statist. Comput. 2, pp 1-4, 1981.

[5] Freund, R. W., Nachtigal, N. M., *A new Krylov-subspace method for symmetric indefinite linear systems*, AT&T Numerical Analysis Manuscript, Bell Labs, Murry Hill, NJ, 1994.

[6] Hebermehl, G., Schlundt, R., Zscheile, H., Heinrich, W., *Simulation of Monolithic Microwave Integrated Circuits*, Preprint No. 235, Weierstraß-Institut für Angewandte Analysis und Stochastik im Forschungsverbund Berlin e.V., April 1996.

[7] Hebermehl, G., Schlundt, R., Zscheile, H., Heinrich, W., *Improved Numerical Solutions for the Simulation of Monolithic Microwave Integrated Circuits*, Preprint No. 236, Weierstraß-Institut für Angewandte Analysis und Stochastik im Forschungsverbund Berlin e.V., April 1996.

[8] Paige, C. C., Saunders, M. A., *Solution of Sparse Indefinite Systems of Linear Equations*, SIAM J. Numer. Anal. 12, 4, pp. 617-629, September 1975.

[9] Saad, Y., *SPARSKIT: A basic tool kit for sparse matrix computation*, Techn. Report CSRD TR 1029, CSRD, University of Illinois, Urbana, IL, 1990.

[10] Saad, Y., *Highly parallel preconditioners for general sparse matrices*, in Golub, G., Luskin, M., Greenbaum, editors, *Recent Advances in Iterative*

Methods, IMA Volumes in Mathematics and Its Applications, Vol. 60, pp. 165-199, New York, Springer Verlag, 1994.

[11] Weiland, T., *Three dimensional resonator mode computation by finite difference method*, IEEE Trans. Magn., Vol. MAG-21, pp. 2340-2343, Nov. 1985.

[12] Weiland, T., *On the unique numerical solution of Maxwell eigenvalue problems in three dimensions*, Particle Accelerators, Vol. 17, pp. 227-242, 1985.

[13] Yee, K. S., *Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media*, IEEE Transactions on Antennas and Propagation, Vol. AP-14, No. 3, May 1966.