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Eigen Mode Computation of Microwave and Laser Structures Including PML

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Abstract

The field distribution at the ports of the transmission line structure is computed by applying Maxwell's equations to the structure. Assuming longitudinal homogeneity an eigenvalue problem can be derived, whose solutions correspond to the propagation constants of the modes. The nonsymmetric sparse system matrix is complex in the presence of losses and Perfectly Matched Layer. The propagation constants are found solving a sequence of eigenvalue problems of modified matrices with the aid of the invert mode of the Arnoldi method. Using coarse and fine grids, and a new parallel sparse linear solver, the method, first developed for microwave structures, can be applied also to high dimensional problems of optoelectronics.

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1 Introduction

The fields of applications are mobile communications, radio links, automobile radar systems, optical communications and material processing. The commercial applications of microwave circuits cover the frequency range between 1 GHz and about 100 GHz, special applications in radioastronomy use even higher frequencies up to 1 THz. For optoelectronic devices frequencies about several hundred THz are common.

Basic elements of the structures are their transmission lines, whose propagation behavior has to be determined accurately. The propagation behavior of the transmission lines can be calculated by applying Maxwellian equations to the infinitely long homogeneous transmission line structure and solving an eigenvalue problem [1].

Only a few modes of smallest attenuation are able to propagate and have to be taken into consideration. Using a conformal mapping between the plane of propagation constants and the plane of eigenvalues the task is to compute all eigen modes in a region, bounded by two parabolas. The region is covered by a number of overlapping circles. The eigen modes in these circles are found solving a sequence of eigenvalue problems of modified matrices [2] with the aid of the invert mode of the Arnoldi iteration using shifts.

For numerical treatment, the computational domain has to be truncated by electric or magnetic walls or by a so-called absorbing boundary condition simulating open space. A very efficient formulation for the latter case is the Perfectly Matched Layer (PML) [3]. Introducing the complex, anisotropic material PML leads to an increased computational time.

Due to the fact, that only small fractions of a microwave circuit can be simulated, the pressure to larger problem sizes is evident. Especially, the application of the method for optoelectronic devices requires new strategies to reduce the numerical effort and storage requirement. The computation of large cross sections combined with an extension of specific material layers in the sub μm-range yields high dimensional problems. Additionally, due to the high wavenumber in semiconductor lasers the region containing potential propagating modes grows substantially. That means, a significant higher number of eigenvalue problems have to be solved. To reduce the execution times, in a first step the problem is solved using a coarse grid in order to find approximately the locations of the interesting propagation constants. The accurate modes are calculated in a second step for an essentially reduced region using a fine grid. In addition, the method is optimized reducing the storage requirement and the computing times applying a new linear sparse solver, that can be used serial or parallel.

2 Boundary Value Problem

We start from a three-dimensional structure. The structure under investigation can be described as an interconnection of infinitely long transmission lines. The junction, the so-called discontinuity, may have an arbitrary structure. The transmission lines have to be longitudinal homogeneous. Ports are defined on the transmission lines. A three-dimensional boundary value problem can be formulated using the integral form of Maxwell's equations in the frequency domain in order to compute the electromagnetic field:

$$\oint_{\partial\Omega} \vec{H} \cdot d\vec{s} = \int_{\Omega} \jmath\omega[\epsilon]\vec{E} \cdot d\vec{\Omega}, \qquad \oint_{\cup\Omega} ([\epsilon]\vec{E}) \cdot d\vec{\Omega} = 0, \tag{1}$$

$$\oint_{\partial\Omega} \vec{E} \cdot d\vec{s} = -\int_{\Omega} \jmath\omega[\mu]\vec{H} \cdot d\vec{\Omega}, \qquad \oint_{\cup\Omega} ([\mu]\vec{H}) \cdot d\vec{\Omega} = 0, \tag{2}$$

$$\vec{D} = [\epsilon]\vec{E}, \ \ \vec{B} = [\mu]\vec{H}, \ \ [\epsilon] = \mathrm{diag}\left(\epsilon_x, \epsilon_y, \epsilon_z\right), \ \ [\mu] = \mathrm{diag}\left(\mu_x, \mu_y, \mu_z\right). \tag{3}$$

The transverse electric mode fields at the ports are the solutions of an eigenvalue problem for the transmission lines. All other parts of the surface of the computation domain are assumed to be an electric or a magnetic wall. The PML's are filled with an artificial material with complex anisotropic material properties. Therefore, the quantities are diagonal complex tensors.

3 Maxwellian Grid Equations

The Maxwellian equations are discretized using staggered nonequidistant rectangular grids. Using the Finite Integration Technique (FIT) [4], [5], [6] with the lowest order integration formulae

$$\oint_{\partial\Omega} \vec{f} \cdot d\vec{s} \approx \sum(\pm f_i s_i), \quad \int_{\Omega} \vec{f} \cdot d\vec{\Omega} \approx f\Omega \tag{4}$$

equations (1), (2) are transformed into a set of Maxwellian grid equations

$$A^T D_{s/\mu}\vec{b} = \jmath\omega\epsilon_0\mu_0 D_{A_\epsilon}\vec{e}, \qquad B D_{A_\epsilon}\vec{e} = 0, \tag{5}$$

$$A D_s \vec{e} = -\jmath\omega D_{A_\mu}\vec{b}, \qquad \tilde{B} D_{A_\mu}\vec{b} = 0. \tag{6}$$

The vectors $\vec{e}$ and $\vec{b}$ contain the components of the electric field intensity and the magnetic flux density of the elementary cells, respectively. The diagonal matrices $D_{s/\mu}$, D_{A_ϵ}, D_s, and D_{A_μ} contain the information on cell dimension and material. A, B, and $\tilde{B}$ are sparse.

Eliminating the components of the magnetic flux density from the two equations of the left-hand side of (5), (6) we get the system of linear algebraic equations

$$(A^T D_{s/\mu} D_{A_\mu}^{-1} A D_s - k_0^2 D_{A_\epsilon})\vec{e} = 0, \quad k_0 = \omega\sqrt{\epsilon_0\mu_0}, \tag{7}$$

which have to be solved using the boundary conditions. k_0 is the wavenumber in vacuum.

4 Eigen Value Problem

The field distribution at the ports is computed assuming longitudinal homogeneity for the transmission line structure. Thus, any field can be expanded into a sum of so-called modal fields which vary exponentially in the longitudinal direction

$$\vec{E}(x, y, z) = \underline{\vec{E}}(x, y) e^{\mp \jmath k_z z}. \tag{8}$$

A substitution of ansatz (8) into the system of linear algebraic equations (7) and the elimination of the longitudinal electric field intensity components by means of the electric-field divergence equation $BD_{A_\epsilon}\vec{e} = 0$ (see (5)) gives an eigenvalue problem

$$C\underline{\vec{e}} = \gamma\underline{\vec{e}}, \quad \gamma = -4\sin^2(hk_z). \tag{9}$$

$\underline{\vec{e}}$ consists of components of the discretized eigenfunctions $\underline{\vec{E}}$. $2h$ is the length of an elementary cell in z-direction. The sparse matrix C is in general nonsymmetric complex. The order of C is $n = 2n_x n_y - n_b$. $n_x n_y$ is the number of elementary cells at the port. The size n_b depends on the number of cells with perfectly conducting material. The relation between the propagation constants k_z and the eigenvalues γ is nonlinear, and can be expressed as

$$k_z = \frac{\jmath}{2h} \ln\left(\frac{\gamma}{2} + 1 + \sqrt{\frac{\gamma}{2}\left(\frac{\gamma}{2} + 2\right)}\right) = \beta - \jmath\alpha. \tag{10}$$

We are interested only in a few modes with the smallest attenuation. These are the modes with the smallest magnitude of imaginary part, but possibly with large real part of their propagation constant. The computation of all eigenvalues in order to find a few propagation constants must be avoided for the high-dimensional problem. For numerical treatment we have to limit the search for propagation constants by a maximum value k_f of their real part. This k_f value depends on the highest permittivity $[\epsilon]$ and permeability $[\mu]$ values of the waveguide, though regions with metallic or PML filling are ignored, see [2]. Using the limited k_f and a preset maximum value α_m of the imaginary part of the propagation constants the region containing the interesting constants is defined as a rectangle $\hat{F}$ bounded by the lines

$$\beta = \pm k_f \quad \text{and} \quad \alpha = \alpha_m. \tag{11}$$

In an additional step all computed modes that are related to the PML boundary are neglected, using the power part criterion given with [8]. We can use the approximation $\sin(x) \approx x$ in (9) if we choose h to be small enough, which is necessary anyway to get small discretization errors:

$$\gamma = -4\sin^2(hk_z) \approx -4(hk_z)^2 = u + \jmath v. \tag{12}$$

With aid of the approximation (12) we get a conformal mapping between the plane of eigenvalues (γ-plane) and the plane of propagation constants (k_z-plane, see (10)):

$$u = -4h^2(\beta^2 - \alpha^2), \quad v = 8h^2\alpha\beta. \tag{13}$$

Using this mapping the rectangle $\hat{F}$ of the k_z-plane is transformed into a region F of the γ-plane bounded by the two parabolas

$$v = \pm 4hk_f\sqrt{u + 4h^2{k_f}^2} \quad \text{and} \quad v = \pm 4h\alpha_m\sqrt{-u + 4h^2{\alpha_m}^2}. \tag{14}$$

That means, we have to find all eigenvalues of the region bounded by the parabolas.

5 Computation of Eigen Modes

We need an algorithm that computes just a few selected eigenvalues and eigenvectors of a complex sparse matrix. A state-of-the-art algorithm for such problems is the Arnoldi method [9], [10]. In general the Arnoldi method converges for our problem only using the invert mode and looking for eigenvalues of largest magnitude. Thus, a simple way to find the eigenvalues located in the region F would be to look for all eigenvalues of smallest magnitude, which are located in a circle centered on the origin and covering the region F. Caused by the high wavenumber k_f, the number of eigenvalues located in this circle is too much in general for a feasible computation using an iterative method. We can solve this problem covering the region F with $s \geq 1$ circles C_i, $i = 1(1)s$, centered on the u-axis and calculating the eigenvalues located in these circles. That is done in the following way. s points

$$\hat{P}_i(\beta_i, \alpha_m), \quad i = 1(1)s, \quad \beta_1 = \frac{k_f}{s} \geq \bar{\beta}, \quad \beta_s = k_f, \quad \text{with} \quad \bar{\beta} = \sqrt{3}\alpha_m \tag{15}$$

are defined on the interval $[0, k_f]$ of the line $\alpha = \alpha_m$. The distance between the points have not to be equidistant and is controlled as shown below. Even the meaning of the distance $\bar{\beta}$ is discussed below. The points $\hat{P}_i$ are transformed into the points P_i of the γ-plane. They are located on the parabola ((14), right formula). The s circles C_i of the γ-plane

$$(u + m_i)^2 + v^2 = {r_i}^2, \;\; r_i = \sqrt{(\Im(P_i))^2 + (m_i - \Re(P_i))^2}, \quad i = 1(1)s, \tag{16}$$

with

$$m_1 = 0, \;\; m_i = \frac{(\Re(P_{i+1}))^2 - (\Re(P_i))^2 + (\Im(P_{i+1}))^2 - (\Im(P_i))^2}{\Re(P_{i+1}) - \Re(P_i)} \tag{17}$$

are centered on the u-axis, covering the region bounded by the parabolas.

In order to find all eigenvalues, located in the circle C_i, l points Q_j are defined on the periphery of C_i. The matrix C is extended by the diagonal matrix Q. The diagonal elements of Q are the l complex elements Q_j:

$$\bar{C} = \begin{pmatrix} Q & \\ & C \end{pmatrix}, \quad Q = diag(Q_1, ..., Q_l). \tag{18}$$

The s eigenvalue problems

$$(\bar{C} - m_i I)\underline{\vec{e}} = (\gamma - m_i)\underline{\vec{e}}, \quad i = 1(1)s, \tag{19}$$

are solved with the aid of the implicitly restarted Arnoldi method using the invert mode. The eigenvalue problems can be solved separably.

The number m of eigenvalues to be computed for this circle must be l on the first call to the Arnoldi procedure. The main idea is to raise m by l for so long until at least one value Q_j was found. But, since $m \ll \bar{n}$ ($\bar{n}$ order of matrix $\bar{C}$) for a feasible computation, one has to restrict the number m of required eigenvalues by m_{max}. If m exceeds m_{max}, we insert a point $\hat{P}_{i+\frac{1}{2}}$ between $\hat{P}_i$ and $\hat{P}_{i+1}$ and restart with $m = l$. The same procedure is used if a given number ν_{max} of iterations in the Arnoldi method is exceeded. If the condition

$$\Delta\hat{P} = \Re(\hat{P}_{i+\frac{1}{2}}) - \Re(\hat{P}_i) \geq \frac{\alpha_m}{2} \tag{20}$$

cannot be fulfilled, we have to restart with new parameters m_{max}, ν_{max} and possibly α_m.

If all eigenvalues Q_j are found in case of $m > l$, we look for the eigenvalue γ_{max} of largest magnitude. If $\sqrt{|\gamma_{max}|} > r_i$, a new circle $\tilde{C}_i$ of radius $\sqrt{|\gamma_{max}|}$ with the same center as C_i is defined. The left intersection point of this circle with the parabola ((14), right formula) is used as new point P_{i+1}, and $\Delta\hat{P} = \Re(\hat{P}_{i+1}) - \Re(\hat{P}_i)$ as distance for the next step. m is reduced by the number of eigenvalues with $\sqrt{|\gamma|} > r_i$ for the next circle.

Separating the new values on each eigenvalue problem i, we are sure to have found all eigenvalues which are located in the corresponding circles C_i. Applying the mapping (13) the circles C_i (see (16)) are transformed into Cassinian curves $\hat{C}_i$

$$(\beta^2 + \alpha^2)^2 - \frac{m_i}{2h^2}(\beta^2 - \alpha^2) = \frac{{r_i}^2}{16h^4} - \frac{{m_i}^2}{16h^4}, \tag{21}$$

which cover the rectangle $\hat{F}$ containing all desired propagation constants. Propagation constants outside of $\hat{F}$ and PML-Modes are eliminated. The Cassinian curves $\hat{C}_i$, $i = 2(1)s$, consist of two separated ovals, if $r_i < m_i$. Using $\bar{\beta}$ as minimum distance between two points $\hat{P}_i$ and $\hat{P}_{i+1}$ (see (15)) other shapes of Cassinian curves (e.g. waisted ovals), which would lead to higher execution times, are avoided.

6 Optoelectronic Devices

The maximum cell size of discretization should be less than $\frac{\lambda}{10}$, where λ denotes the wavelength in the material with the highest $\Re(\epsilon)$. Essentially finer grids have to be used for regions of the circuit with highly variable electric fields. That means, the problems become high dimensional, and only small fractions of a circuit can be simulated. Especially the application of the method to optoelectronic devices requires new strategies. The dimension of the eigenvalue problem to be solved increases essentially in this case caused by the short wavelength. In addition, due to the high

wavenumber in optoelectronic devices the length of the rectangle $\hat{F}$ containing potential propagation constants grows substantially. That means, we have to calculate a significant higher number of eigenvalue problems. Due to electric and magnetic walls behind the PML undesired modes are generated inside the computation domain. The non physical modes can be eliminated by examining the eigenfunctions. Anyway, the number of eigen modes to be calculated increases caused by the shifted modes. Due to the significant difference between the magnitude of the real and imaginary part of the propagation constant a high computational accuracy has to be required. To overcome these problems two strategies have been realized.
(1) To reduce the execution times, in a first step the problem is solved using a coarse grid with lower accuracy requirements in order to find approximately the locations of the interesting propagation constants. Finally the modes are calculated in a second step for an essentially reduced region using a fine grid, that fulfills higher accuracy requirements.
(2) Because in general the Arnoldi method does not converge using the regular mode for our eigenvalue problem the invert mode with shifting (see (19)) is applied. A time and memory consuming system of linear algebraic equations has to be solved on each iteration step in this case. The storage requirement and the computing times could be reduced substantially applying the new linear sparse solver PARDISO [11], [12] rather than the formerly used UMFPACK [13]. The fill in is reduced approximately by a factor of 4.75. Moreover, the dynamic memory allocation of PARDISO allows to diminish the memory requirements. The computing times for the numerical factorization and forward and backward solve are reduced on the average by a factor of 15 and 4 for our problem, respectively. The algorithm is split into three phases: symbolic factorization, numerical factorization, and forward and backward solve. The symbolic factorization can be used for all modified matrices of our problem. The numerical factorization has to be repeated for every new shift.
The typical ratio of factorization time to solution time on a single CPU can be used to define ν_{max} in the subinterval control process (see section 5). This ratio amounts on the average 20. That means, the costs using $\nu_{max} = 60$ Arnoldi iterations for the computation of m eigen modes in a circle C_i defined by the points P_i, P_{i+1} are comparable with the costs, defined by the costs for two circles defined by the points $P_i, P_{i+\frac{1}{2}}$ and $P_{i+\frac{1}{2}}, P_{i+1}$ using $\nu_{max} = 20$ iterations. On the other hand the time is lost, interrupting the computation of m eigen modes after $\nu_{max} = 60$ iterations and starting a new iteration process for two reduced circles. Thus, we use a greater ν_{max}. Moreover, due to the significant difference between the length and the height of the rectangular region $\hat{F}$ in the k_z-plane we have to solve a large number s of eigenvalue problems (see section 7). In order to diminish this number we use Cassinian curves with relatively large diameters. That means, a number of non desired eigenvalues outside of the area $\hat{F}$ has to be calculated. In general the computation of a large number m of eigenvalues in one circle needs more iterations than a small number.

The s eigenvalue problems (19) could be solved independently and in parallel using s processors and single CPU mode of PARDISO. But that means, the amount of memory increases nearly by a factor of s, and the maximum problem size which could be managed is reduced. Contrary to that the parallel CPU mode of PARDISO provides an additional possibility to reduce the computing times for high dimensional problems on shared memory multiprocessors without essential additional memory requirements.

7 Laser Application

As an example we have calculated the guided mode of an optoelectronic device. A so called self aligned stripe (SAS) laser is investigated, see Figure 1. This laser structure contains an additional, so called antiguided layer (marked with $\epsilon_x = 12 - i * 0.1$ in Figure 1) outside the emitting stripe (marked with $\epsilon_x = 11.3 + i * 0.05$ in Figure 1). This high power laser diode excites only the fundamental mode, the active region is useful for wavelengths shorter than 800 nm. The frequency is fixed to $299.7925 * 10^{12}$ Hz.

In our eigen mode computation of the laser structure a graded mesh of 283 times 345 elementary cells, including 10-cell PML regions, is used as a fine grid. The maximum cell size amounts $\frac{\lambda}{12} = 25$nm, where λ denotes the wavelength in the material with the highest $\Re(\epsilon)$. The minimum cell size is 1 nm. Maximum cell size is scaled down exponentially in the vertical direction near the 100 nm zones and in the horizontal direction near the material cut 118 and 119 (see Figure 1). The dimension of the eigenvalue problem is 192 423. The eigenvalues and eigenvectors have been solved with the relative accuracy $tol = 10^{-10}$, and with $m_{max} = 16$, $l = 5$ (see section 5). 84 Cassinian curves have been used to cover the long small region of the complex plane ($\alpha_m = 2500\,\mathrm{m}^{-1}$, $k_f = 21\,765\,592\,\mathrm{m}^{-1}$, see (11)) containing potential guided modes. A maximum number $\nu_{max} = 120$ of Arnoldi iteration has been used. The total computational time amounts approximately 3h and 23 minutes using a Compaq Professional Workstation with processor XP1000 alpha 667 MHz.

One guided mode according to the lasers fundamental mode, was found. The computed complex propagation constant is given by $k_z = 20\,817\,578 + j\,1\,488$.

A graded mesh of 121 times 127 elementary cells is used as a coarse grid. The maximum cell size amounts 80nm, and the minimum cell size 4nm. The dimension of the eigenvalue problem is 29 625. The total computational time amounts approximately 19 minutes using the relative accuracy $tol = 10^{-7}$. The circle that contains the guided mode is known after this step. The time to find the accurate value k_z using the fine grid amounts only 142 s. Thus, the computational time is reduced by a factor of 1/9 for the given structure.

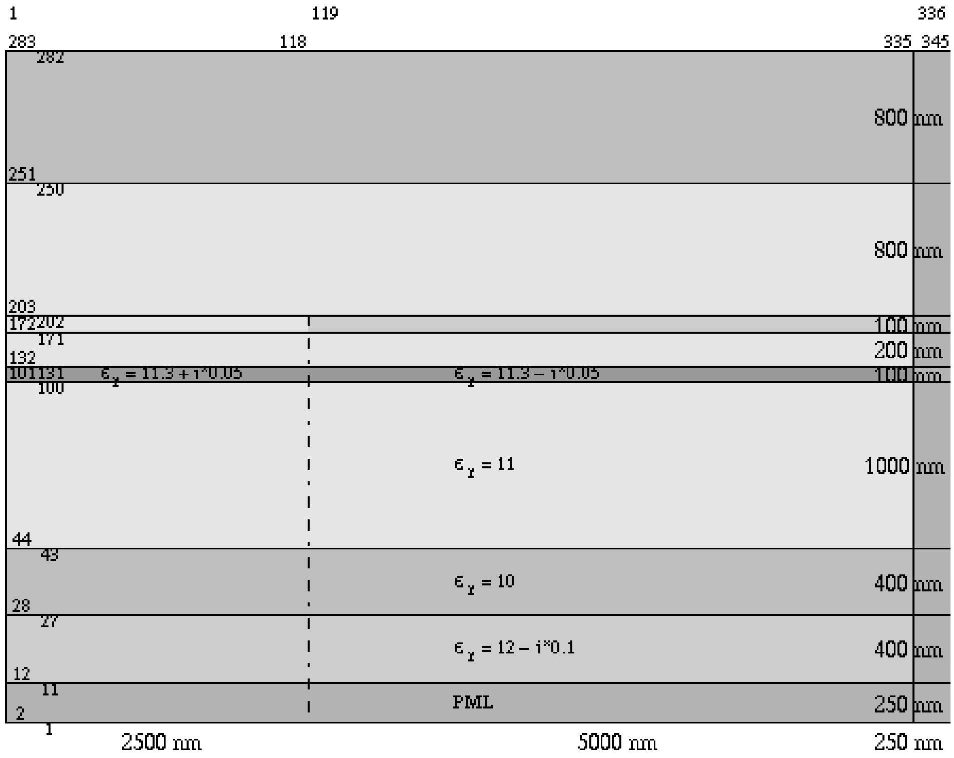

Figure 1: Laser (amplifier)

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