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Numerical Techniques in the Simulation of Microwave and Laser Structures Including PML

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Abstract

The properties of circuit structures can be described in terms of their scattering matrix. For the simulation of these structures, we use a Finite Difference Frequency Domain (FDFD) method in order to solve the three dimensional boundary value problem, governed by Maxwells equations. For the computation of the discrete grid equations, advanced preconditioning techniques are applied to reduce the dimension and the number of iterations solving the large-scale systems of linear algebraic equations by means of a block Krylov subspace method. The computational domain is truncated by electric or magnetic walls, open structures are treated using the Perfectly Matched Layer (PML) absorbing boundary condition. Calculating the excitation at the structures ports, one obtains an eigenvalue problem and thus large-scale systems of linear algebraic equations. The interesting modes of smallest attenuation are found solving a sequence of eigenvalue problems of modified matrices. Non-physical PML modes are detected by checking the eigenfunctions. Due to the high wavenumbers that have to be treated in optoelectronic device simulations, the number of modified eigenvalue problems as well as the dimension of the problem grows substantially in comparison to microwave structures. To reduce the execution times a coarse and a fine grid and parallelization techniques are used.

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1 Introduction

The subject under investigation are passive structures of arbitrary geometry. They are connected to the remaining circuit by transmission lines and described by the scattering matrix. In order to characterize their electrical behaviour, infinite long transmission lines are assumed at the ports (see Figure 1). The scattering matrix describes the structure in terms of wave modes on the transmission line sections at the ports. One can extract this matrix from the orthogonal decomposition of the electric field at two neighboring cross-sectional planes on each transmission line for a number of linearly independent excitations.

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 [1] and subsequently the scattering matrix. At the ports the transverse electric field is given by superposing transmission line modes. The transverse electric mode fields are the solutions of an eigenvalue problem for the transmission lines [2]. On all other parts of the surface of the computation domain the tangential electric or magnetic field is assumed to be equal zero. In order to simulate open structures we use the uniaxial Perfectly Matched Layer formulation [3] as an absorbing boundary condition.

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 eigen modes are found solving a sequence of eigenvalue problems of modified matrices [5]. The resulting nonsymmetric sparse system matrix is complex in the presence of losses and Perfectly Matched Layers. The method, developed initially for a reliable calculation of all complex eigenvalues from microwave structure computations [5], is expanded to meet the very special requirements of optoelectronic structure calculations. Relatively large cross sections and highest frequencies yields increased dimensions and numbers of eigenvalue problems. Using the results of a coarse grid calculation within the final fine grid calculation yields a remarkable reduced numerical effort. The use of a parallelized solver results in an additional speed up of computation time.

The electromagnetic fields and the scattering matrix elements are computed by the solution of large-scale systems of linear equations with indefinite complex symmetric coefficient matrices. In general, these matrix problems have to be solved repeatedly for different right-hand sides, but with the same coefficient matrix. The number of right-hand sides depends on the number of ports and modes. The systems of linear equations are solved using a block Krylov subspace iterative method. Independent set orderings, Jacobi and SSOR preconditioning techniques are applied to reduce the dimension and the number of iterations [6].

In general, the computation of the eigenvalue problem and of the system of linear algebraic equations have to be done for several frequencies.

2 Scattering Matrix

The incoming modes $a_{\sigma,\nu}$ are reflected and transmitted at the discontinuity. The resulting outgoing modes are denoted by $b_{\rho,\nu}$. The scattering matrix

$$S = (S_{\rho,\sigma}), \quad b_{\rho,\nu} = \sum_{\sigma=1}^{m_s} S_{\rho,\sigma} a_{\sigma,\nu}, \quad \nu, \rho, \sigma = 1(1)m_s, \tag{1}$$

$$\text{with} \quad m_s = \sum_{p=1}^{\overline{p}} m^{(p)}, \quad \rho = l + \sum_{q=1}^{p-1} m^{(q)} \tag{2}$$

describes the structure in terms of wave modes on the transmission line sections at the ports. $m^{(p)}$ denotes the number of modes which have to be taken into account at the port p. $\overline{p}$ is the number of ports. The modes on a port p are numbered with l. 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 $p + \Delta p$ on each waveguide for a number of linear independent excitations of the transmission lines.

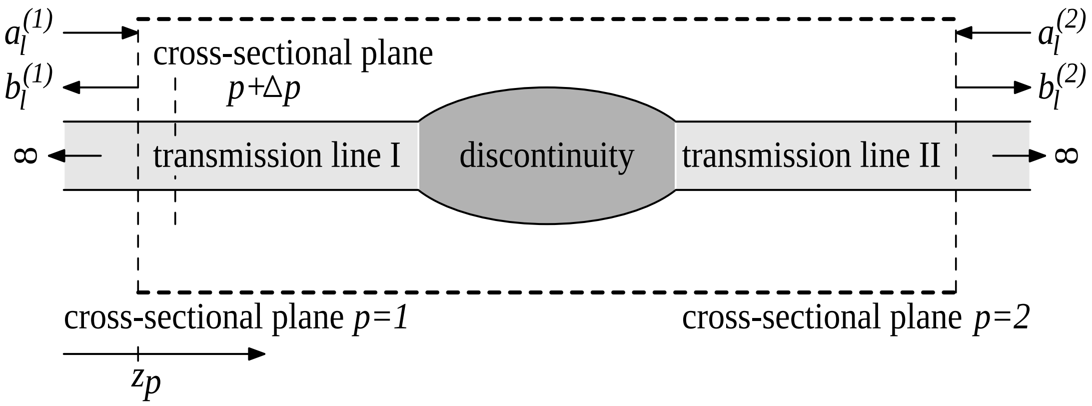

Figure 1: Structure under investigation

3 Boundary Value Problem

The electromagnetic field is computed using a three dimensional boundary value problem. We start from Maxwell's equations in the frequency domain, written in integral form,

$$\begin{aligned}
\oint_{\partial\Omega} \vec{H} \cdot d\vec{s} &= \int_{\Omega} \jmath\omega[\epsilon]\vec{E} \cdot d\vec{\Omega}, \\
\oint_{\partial\Omega} \vec{E} \cdot d\vec{s} &= -\int_{\Omega} \jmath\omega[\mu]\vec{H} \cdot d\vec{\Omega}, \\
\oint_{\cup\Omega} ([\epsilon]\vec{E}) \cdot d\vec{\Omega} &= 0, \\
\oint_{\cup\Omega} ([\mu]\vec{H}) \cdot d\vec{\Omega} &= 0
\end{aligned} \tag{3}$$

with the constitutive relations

$$\begin{aligned}
\vec{D} = [\epsilon]\vec{E}, \quad [\epsilon] = \mathrm{diag}\left(\epsilon_x, \epsilon_y, \epsilon_z\right), \\
\vec{B} = [\mu]\vec{H}, \quad [\mu] = \mathrm{diag}\left(\mu_x, \mu_y, \mu_z\right).
\end{aligned} \tag{4}$$

With the PML regions being filled with a complex anisotropic material, diagonal complex tensors have to be introduced, describing this artificial material.

At the ports p the transverse electric field $\vec{E}_t(z_p)$ is given by superposing transmission line modes $\vec{E}_{t,l}(z_p)$. On all other parts of the computation domains surface the tangential electric or magnetic field is assumed to be equal to zero:

$$\vec{E}_t(z_p) = \sum_{l=1}^{m^{(p)}} w_l(z_p)\vec{E}_{t,l}(z_p), \quad \vec{E} \times \vec{n} = 0, \;\; \vec{H} \times \vec{n} = 0. \tag{5}$$

The transverse electric mode fields are the solutions of an eigenvalue problem for the transmission lines (see section 4).

The problem is solved numerically by the Finite Difference Method in Frequency Domain (FDFD) [1]. Staggered nonequidistant rectangular grids are used. Using the lowest-order integration formulae

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

Maxwell's equations are transformed into a set of Maxwellian grid equations [4]:

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

The vectors $\vec{e}$ and $\vec{b}$ contain the components of the electric field $\vec{E}$ and of the magnetic flux density $\vec{B}$ 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 dimensions and material properties. A, B and $\tilde{B}$ are sparse and contain the values 1, -1 and 0 only. Substituting the components of the magnetic flux density from the two equations of the left-hand sides of (7) the number of unknowns can be reduced by a factor of two and we get the system of linear algebraic equations

$$(A^T D_{s/\mu} D_{A_\mu}^{-1} A D_s - k_0^2 D_{A_\epsilon})\vec{e} = 0, \quad k_0 = \omega\sqrt{\epsilon_0\mu_0}, \tag{8}$$

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

4 Eigenvalue Problem

Assuming the transmission lines to be longitudinally homogeneous any field can be expanded into a sum of modal fields which vary exponentially in the longitudinal direction:

$$\vec{E}(x, y, z \pm 2h) = \vec{E}(x, y, z)e^{\mp \jmath k_z 2h}. \tag{9}$$

k_z is the propagation constant. $2h$ is the length of an elementary cell in z-direction. We consider the field components in three consecutive elementary cells. The electric field components of the vector $\vec{e}$ (see (8)) $E_{x_{i,j,k+1}}$, $E_{x_{i,j,k-1}}$, $E_{y_{i,j,k+1}}$, $E_{y_{i,j,k-1}}$, $E_{z_{i,j,k-1}}$, $E_{z_{i+1,j,k-1}}$, and $E_{z_{i,j+1,k-1}}$ are expressed by the values of cell k using ansatz (9). The longitudinal electric field components E_z can be eliminated by means of the electric-field divergence equation $BD_{A_\epsilon}\vec{e} = 0$ (see (7)). Thus, we get an eigenvalue problem for the transverse electric field $\underline{\vec{e}}$ on the transmission line region:

$$C\underline{\vec{e}} = \gamma\underline{\vec{e}}, \quad \gamma = -4\sin^2(hk_z). \tag{10}$$

The relation between the eigenvalues γ and the propagation constants k_z is nonlinear:

$$k_z = \frac{\jmath}{2h}\ln\left(\frac{\gamma}{2} + 1 + \sqrt{\frac{\gamma}{2}\left(\frac{\gamma}{2} + 2\right)}\right) = \beta - \jmath\alpha. \tag{11}$$

We are interested only in 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. A reasonable estimation of this maximum value is derived for the lossy case including PML for inhomogeneously filled waveguides in [7]:

$$\Re(k_z) \leq k_f = \omega\Re(\sqrt{\epsilon_m\mu_m}). \tag{12}$$

ϵ_m and μ_m are properties of the material that yields the largest value of the right-hand side of Equation (12). 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

$$\beta = \pm k_f \quad \text{and} \quad \alpha = \pm\alpha_m. \tag{13}$$

We can use the approximation

$$\gamma = -4\sin^2(hk_z) \approx -4(hk_z)^2 = u + \jmath v \tag{14}$$

in (10) if we choose h to be small enough. With aid of the approximation (14) we get a conformal mapping between the plane of eigenvalues (γ-plane) and the plane of propagation constants (k_z-plane, see (11)):

$$u = -4h^2(\beta^2 - \alpha^2), \quad v = 8h^2\alpha\beta. \tag{15}$$

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

$$\begin{aligned} v &= \pm 4hk_f\sqrt{u + 4h^2{k_f}^2}, \\ v &= \pm 4h\alpha_m\sqrt{-u + 4h^2{\alpha_m}^2}. \end{aligned} \tag{16}$$

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

In an additional step all computed modes that are related to the PML boundary are neglected, using the power part criterion given with [8].

5 Computation of Propagation Constants

The dimension n of the eigenvalue problem (10) is too large to use a direct method. We need an iterative 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. Especially, due to the high wavenumber in optoelectronic devices the potential modes of smallest attenuation are located in a longsome region F (see (16)). That means, also the two step procedure covering the region $\hat{F}$ by a circle and a lemniscate (see [7]) cannot be applied in this case. Thus, we 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

$$\hat{P}_i(\beta_i, \alpha_m), \ \ \beta_1 = \frac{k_f}{s} \geq \bar{\beta}, \ \ \beta_s = k_f, \ \ \bar{\beta} = \sqrt{3}\alpha_m \tag{17}$$

are defined on the interval $[0, k_f]$ of the line $\alpha = \alpha_m$. 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 ((16), second formula). The s circles C_i of the γ-plane

$$(u + m_i)^2 + v^2 = {r_i}^2, \quad r_i = \sqrt{(\Im(P_i))^2 + (m_i - \Re(P_i))^2}, \quad i = 1(1)s, \tag{18}$$

with

$$m_1 = 0, \quad m_i = \frac{(\Re(P_{i+1}))^2 - (\Re(P_i))^2 + (\Im(P_{i+1}))^2 - (\Im(P_i))^2}{\Re(P_{i+1}) - \Re(P_i)} \tag{19}$$

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:

$$\bar{C} = \begin{pmatrix} Q & \\ & C \end{pmatrix}, \quad Q = diag(Q_1, ..., Q_l). \tag{20}$$

The s eigenvalue problems

$$(\bar{C} - m_i I)\underline{\vec{e}} = (\gamma - m_i)\underline{\vec{e}}, \quad i = 1(1)s, \tag{21}$$

are solved by means of the implicitly restarted Arnoldi method using the invert mode. The number m of eigenvalues to be computed for one circle must be l on the first call to the Arnoldi procedure. The main idea is to increase an increment m by l as long as at least one value Q_j is found. The eigenvalue problems can also be computed for subintervals defined by

$$i = i_1(1)i_2 \ \text{ or } \ i = i_2(-1)i_1, \ \ 1 \le i_1 < i_2 \le s. \tag{22}$$

The distance between the points have not to be equidistant and is controlled. 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

$$\Delta\hat{P} = \Re(\hat{P}_{i+\frac{1}{2}}) - \Re(\hat{P}_i) \ge \frac{\alpha_m}{2} \tag{23}$$

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 ((16), second 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 mapping (15) the circles C_i (see (18)) are transformed into Cassinian curves $\hat{C}_i$

$$(\beta^2 + \alpha^2)^2 - \frac{m_i}{2h^2}(\beta^2 - \alpha^2) = \frac{{r_i}^2}{16h^4} - \frac{{m_i}^2}{16h^4}, \tag{24}$$

which cover the rectangle containing all desired propagation constants. Propagation constants outside of the rectangle and PML related 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 (17)) other shapes of Cassinian curves (e.g. waisted ovals), which would lead to higher execution times, are avoided.

Because the invert mode of the Arnoldi method is used a time and memory consuming system of partly ill-conditioned nonsymmetric complex linear algebraic equations has to be solved on each iteration step. The linear sparse solver PARDISO [11], [12] is applied in order to fulfill the high accuracy requirements of the eigenvalue problem, and to reduce the computing times in comparison to the formerly used UMFPACK [13]. Additionally, the dynamic memory allocation of PARDISO allows to diminish the memory requirements. 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 factorization is applied to matrix C. The diagonal matrix Q (see (20)) is considered in the forward and backward solve phase.

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. 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, we have a significant difference between the length and the height of the rectangular region $\hat{F}$ in the k_z-plane in case of high wavenumbers. Consequently, a large number s of eigenvalue problems has to be solved. 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 number s of eigenpairs to be computed depends on the frequency ω. 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 these kinds of structures only a few separate eigenvalue problems have to be solved within our algorithm. Hence a single CPU calculation is almost sufficient.

6 Application to Optoelectronic Devices

For optoelectronic devices frequencies about several hundred THz are common. The region containing potential propagating modes grows substantially. A significant higher number of eigenvalue problems have to be solved within our algorithm. Additionally, the maximum cell size of the discretization should be less than $\frac{\lambda}{10}$, where λ denotes the wavelength in the material with the highest $\Re(\epsilon)$. Additional mesh refinements have to be used for structure regions with highly varying fields. Besides, large cross sections are common for the waveguides under investigation. Thus high dimensional problems have to be handled.

In addition, due to electric and magnetic walls terminating the PML regions, undesired modes are generated inside the computation domain. These non-physical modes can be detected by examining the eigenfunctions. Anyway, the number of eigen modes to be calculated increases because of 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 is required. That means, the numerical effort increases significantly.

To overcome these problems we benefit from two properties. First, the few interesting modes are located in a partial region of the longsome rectangle F, and only the corresponding eigenpairs have to be computed with high accuracy. Second, the eigenvalue problems can be solved separately. Thus, 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. Anyway, the number of modified eigenvalue problems to be solved is high. Thus, we split the interval $[0, k_f]$ (see (17)) into subintervals (see (22)), and compute the corresponding eigenpairs independently and in parallel, for instance on different workstations or shared memory multiprocessors.

Finally the interesting modes are calculated in a second step for an essentially reduced region described by (22) using a fine grid, that fulfills higher accuracy requirements. The parallel CPU mode of PARDISO provides the additional possibility to reduce the computing times for high dimensional problems on shared memory multiprocessors without essential additional memory requirements.

7 Semiconductor Laser Example

As an example we have calculated the guided mode of an optoelectronic device which leads to a more moderate dimension of the corresponding eigenvalue problem. A so called self aligned stripe (SAS) laser is investigated (see Figure 2). The laser structure contains an additional, antiguided layer outside the emitting stripe. 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.

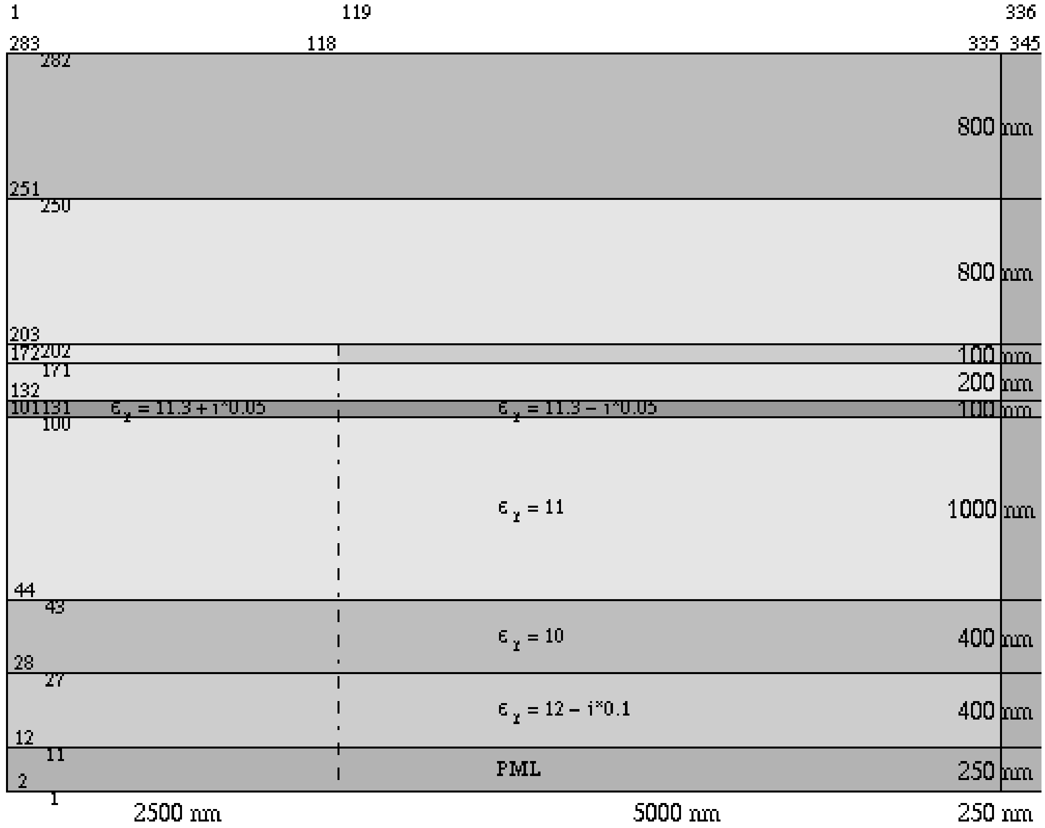

Figure 2: Laser (amplifier)

A graded mesh of 121 times 127 elementary cells, including 10-cell PML regions, is used as a coarse grid. The maximum cell size amounts 80 nm, and the minimum cell size 4 nm. Maximum cell size is scaled down exponentially in the vertical direction near the emitting zone and in the horizontal direction near the material cut at the end of the active zone. The dimension of the eigenvalue problem is 29 625. 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 (13)) containing potential guided modes. The eigenpairs have been computed with the relative accuracy $tol = 10^{-7}$, and with $m_{max} = 16$, $l = 5$ (see section 5). A maximum number $\nu_{max} = 120$ of Arnoldi iteration has been used. The total computational time amounts approximately 1 145 s. One guided mode according to the lasers fundamental mode, was found. The circle that contains the guided mode is known after this step. The computed complex propagation constant is given by $k_z = 20\,818\,302 + j\,1\,401$ using this coarse grid.

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 $\frac{\lambda}{12} = 25\,\mathrm{nm}$, where λ denotes the wavelength in the material with the highest $\Re(\epsilon)$. The minimum cell size is 1 nm. The dimension of the eigenvalue problem is 192 423. The eigenpairs have been calculated with the relative accuracy $tol = 10^{-10}$. The time to find the accurate value of the guided mode in the reduced region using the fine grid amounts only 70 s.

The computed complex propagation constant is given by $k_z = 20\,817\,578 + j\,1\,488$ using the fine grid.

Applying only the fine grid for the long small region on a single CPU the total computational time amounts approximately 3 h and 23 minutes. Thus, the computational time is reduced by a factor of 10 using a coarse and a fine grid. A Compaq Professional Workstation with processor XP1000 alpha 667 MHz has been used for the computations.

Splitting the interval $[0, k_f]$ into q subintervals (see (22)) and solving the corresponding eigenvalue problems in parallel the time for the coarse grid computation is reduced by a factor of q. Additionally, applying the parallel CPU mode of PARDISO to the fine grid computation in the reduced region the computing times for LU decomposition and and for the solve phase could be reduced to 68% and 86%, respectively, using two processors.

8 System of Linear Algebraic Equations

Multiplying (8) by $D_s^{1/2}$ yields a symmetric form of linear algebraic equations:

$$\bar{A}\vec{x} = 0, \quad \bar{A} = (D_s^{1/2} A^T D_{s/\mu} D_{A_\mu}^{-1} A D_s^{1/2} - k_0^2 D_{A_\epsilon}) \tag{25}$$

with $\vec{x} = D_s^{1/2}\vec{e}$. Four kinds of preconditioning and a block quasi-minimal residual algorithm are applied to solve the large scale systems of linear algebraic equations. Details are given with [6].

The gradient of the electric field divergence (see (3))

$$[\epsilon]\nabla([\epsilon]^{-2}\nabla \cdot [\epsilon]\vec{E}) = 0 \tag{26}$$

is equivalent to the matrix equation

$$\bar{B}\vec{x} = 0, \quad \bar{B} = D_s^{-1/2} D_{A_\epsilon} B^T D_{V_{\epsilon\epsilon}}^{-1} B D_{A_\epsilon} D_s^{-1/2}. \tag{27}$$

The diagonal matrix $D_{V_{\epsilon\epsilon}}$ is a volume matrix for the 8 partial volumes of the dual elementary cell. Taking into account the boundary conditions Equations (25) and (27) yields the form

$$\tilde{A}\vec{x} = \vec{b}, \quad \tilde{B}\vec{x} = 0. \tag{28}$$

The effect of the addition of Equations (28) can be interpreted as preconditioning with the preconditioner $(I + \tilde{B}\tilde{A}^{-1})^{-1}$ for system ((28), left equation):

$$(\tilde{A} + \tilde{B})\vec{x} = \vec{b}. \tag{29}$$

$(\tilde{A} + \tilde{B})$ is a complex indefinite symmetric matrix.

In addition, independent set orderings, Jacobi and SSOR preconditioning are applied to accelerate the speed of convergence of the used block Krylov subspace method

[14] for the system of linear algebraic equations (29) that has to be solved with the same coefficient matrix, but multiple right-hand sides. The number m_s (see (2)) of right-hand sides depends on the number of ports and guided modes.

In comparison to the simple lossy case the number of iterations of Krylov subspace methods increases significantly in the presence of Perfectly Matched Layers. The speed of convergence depends on the relations of the edges in a elementary cell of the nonequidistant rectangular grid in this case. The best results can be obtained using cube similar grids. Moreover, overlapping PML conditions on the corners downgrade the properties of the coefficient matrix, and should be avoided. Otherwise, eigenvalues of the matrix are shifted into the negative half plane. That means, the Krylov subspace methods need more iterations.

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