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Abstract

This paper has been motivated by the need for a fast robust adaptive multigrid method to solve the vectorial Maxwell eigenvalue problem arising from the design of optical chips. Our nonlinear multigrid methods are based on a previous method for the scalar Helmholtz equation, which must be modified to cope with the null space of the Maxwell operator due to the divergence condition. We present two different approaches. First, we present a multigrid algorithm based on an edge element discretization of time-harmonic Maxwell's equations, including the divergence condition. Second, an explicit elimination of longitudinal magnetic components leads to a nodal discretization known to avoid discrete *spurious modes* also and a vectorial eigenvalue problem, for which we present a multigrid solver. Numerical examples show that the edge element discretization clearly outperforms the nodal element approach.

AMS Subject Classification: 65N25, 65N30, 65N55

Keywords: Maxwell's equations, eigenvalue problem, edge elements, multigrid methods, waveguide, optical chip design

1 Eigenvalue problems for optical waveguide design

Integrated optical components like semiconductor lasers, optical switches, and filters are essential parts of modern fiber-optical networks, see [7], [8, ch. 2]. Figure 1 shows a mounted MQW-laser of the latest technological generation. Each of them consists of various sub-components, which are connected by waveguides. Therefore, the design of optical waveguides is a central task. The analysis of optical waveguides is based on the knowledge of their guided modes and propagation constants. A schematic representation of an optical chip is given in Fig. 2. The optical beam propagates in z-direction. The geometry of the chip itself is regarded as invariable in this direction. Guided modes are modes that exhibit an

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Figure 1: Si-Submount with MQW laser in material system InGaAsP/InP. (Osram OS)

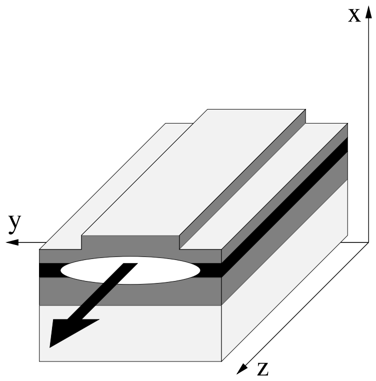

Figure 2: Schematic optical waveguide

intensity distribution invariant in z-direction and with finite lateral extension. In former work we had simplified the basic vectorial Maxwell's equations such that a scalar Helmholtz eigenvalue problem arose [7]. As industrial optical components get more and more complex [17], including sharp and significant jumps in the permittivity of the waveguide materials, this approximation turns out to be too crude. Therefore we have to return to the exact Maxwell's equations as a mathematical model. This leads again to an eigenvalue problem, which, however, is much more complex and is the topic of this paper.

Starting from Maxwell's equations in a source and current free medium and assuming time-harmonic dependence of the electromagnetic field with angular frequency ω the electric and magnetic fields

$$\mathbf{E}(x,y,z,t) = \widetilde{\mathbf{E}}(x,y,z) \cdot \mathrm{e}^{i\omega t},\ \mathbf{H}(x,y,z,t) = \widetilde{\mathbf{H}}(x,y,z) \cdot \mathrm{e}^{i\omega t}$$

must satisfy the time-harmonic Maxwell equations

$$\begin{aligned} \operatorname{curl}\tilde{\mathbf{E}} &= -i\omega\mu\tilde{\mathbf{H}}, & \operatorname{div}\epsilon\tilde{\mathbf{E}} &= 0 \\ \operatorname{curl}\tilde{\mathbf{H}} &= i\omega\epsilon\tilde{\mathbf{E}}, & \operatorname{div}\mu\tilde{\mathbf{H}} &= 0. \end{aligned}$$

Herein $\epsilon = \epsilon(x, y)$ denotes the permittivity and μ the permeability of the material. For simplicity, we assume μ to be constant, $\epsilon = \epsilon_D - i\sigma/\omega$ complex, and drop the wiggles, so that $\tilde{\mathbf{E}} \rightarrow \mathbf{E}$, $\tilde{\mathbf{H}} \rightarrow \mathbf{H}$. From the equations above we then may derive (by direct substitution)

$$\begin{aligned} \operatorname{curl}\epsilon^{-1}\operatorname{curl}\mathbf{H} - \omega^2\mu\mathbf{H} &= 0, \\ \operatorname{div}\mu\mathbf{H} &= 0, \end{aligned} \tag{1}$$

where only the magnetic field is involved. Motivated by the z - invariance of our geometry, we seek solutions of equation (1), which depend harmonically on z, i.e.

$$\mathbf{H}(x, y, z) = \hat{\mathbf{H}}(x, y) \cdot \mathrm{e}^{-ik_z z}.$$

Here k_z is the propagation constant, which is the eigenvalue of interest. In the following, we again drop the hat, so that $\hat{\mathbf{H}} \rightarrow \mathbf{H}$. Let us introduce a reference permittivity ϵ_0, the relative permittivity $\epsilon_r = \epsilon/\epsilon_0$ and the corresponding reference wave number $k_0^2 = \epsilon_0\mu\omega^2$, which is assumed to be given. Upon splitting the magnetic field into a transversal part $\mathbf{H}_\perp(x, y)$ and a longitudinal part $\mathrm{H}_z(x, y)$,

$$\mathbf{H}(x, y) = \mathbf{H}_\perp(x, y) + \mathrm{H}_z(x, y) \cdot \mathbf{e}_z,$$

equation (1) is equivalent to the eigenvalue problem

$$\begin{aligned} \nabla_\perp \times \epsilon_r^{-1}\nabla_\perp \times \mathbf{H}_\perp - k_0^2\mathbf{H}_\perp &= -k_z^2\epsilon_r^{-1}\mathbf{H}_\perp + ik_z\epsilon_r^{-1}\nabla_\perp\mathrm{H}_z & (2) \\ -\nabla_\perp \cdot \epsilon_r^{-1}\nabla_\perp\mathrm{H}_z - k_0^2\mathrm{H}_z &= ik_z\nabla_\perp \cdot \epsilon_r^{-1}\mathbf{H}_\perp & (3) \\ \nabla_\perp \cdot \mathbf{H}_\perp &= ik_z\mathrm{H}_z\,. & (4) \end{aligned}$$

In principle, Maxwell eigenvalue problems divide into two classes. In the so-called *resonance problem*

$$\begin{bmatrix} \nabla_\perp \times \epsilon_r^{-1}\nabla_\perp \times +k_z^2\epsilon_r^{-1} & -ik_z\epsilon_r^{-1}\nabla_\perp \\ -ik_z\nabla_\perp \cdot \epsilon_r^{-1} & -\nabla_\perp \cdot \epsilon_r^{-1}\nabla_\perp \end{bmatrix} \begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{H}_z \end{bmatrix} = k_0^2 \cdot \begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{H}_z \end{bmatrix} \tag{5}$$

we ask for an eigenvalue k_0 or ω, respectively. The structure of this problem is rather simple - the left hand side of equation (5) is a selfadjoint operator in the case of loss-free media and the right hand side consists of a *positive definite mass term.* However, this is not the appropriate problem in integrated optics. There the task is to determine the propagation constant k_z, which appears implicitly in equation (5). By introducing $\mathrm{u}_z = \mathrm{k}_z/i \cdot \mathrm{H}_z$ this so called *waveguide problem* also allows an explicit eigenvalue problem formulation,

$$\begin{aligned} \begin{bmatrix} \nabla_\perp \times \epsilon_r^{-1}\nabla_\perp \times -k_0^2 & \epsilon_r^{-1}\nabla_\perp \\ 0 & -\nabla_\perp \cdot \epsilon_r^{-1}\nabla_\perp - k_0^2 \end{bmatrix} \begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{u}_z \end{bmatrix} &= \\ -k_z^2 \cdot \begin{bmatrix} \epsilon_r^{-1} & 0 \\ \nabla_\perp \cdot \epsilon_r^{-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{u}_z \end{bmatrix}&, \end{aligned} \tag{6}$$

with a non-selfadjoint operator on the left and a *singular* operator on the right hand side. In view of a numerical approximation we have to choose a finite domain of discretization and hence boundary conditions must be prescribed. This is a rather complex issue in the case of optical waveguides, because in many problems boundary conditions are not explicitly given on finite domains. If only *guided modes* are sought, the magnetic field decays exponentially fast to zero outside a finite domain, so we may prescribe zero boundary conditions on a sufficiently large domain.

2 Variational formulations and discretizations

We present two different variational formulations of the system (2)-(4). These two approaches differ by the incorporation of the divergence condition (4) and the treatment of the H_z-component. In the first approach we discretize the transversal components $\mathbf{H}_\perp$ with linear edge elements, H_z with nodal elements and set up a discrete analog of Maxwell's equations. In the second approach we eliminate the H_z-component by the divergence condition and choose a nodal element discretization for $\mathbf{H}_\perp$. For a discussion of these approaches see [10]. In order to avoid confusions with the standard notation for Sobelev spaces we write $\mathbf{u}_\perp$ instead of $\mathbf{H}_\perp$ and introduce $\mathrm{u}_z = 1/i \cdot \mathrm{H}_z$. Recall that ϵ is in general not smooth. So the computational domain may be split up according to

$$\Omega = \Omega_1 \cup ... \cup \Omega_{N},$$

where ϵ is now smooth on each subdomain Ω_i. The boundary between Ω_i and Ω_j is denoted by Γ_{ij}. Furthermore we introduce the inner products by $(\mathbf{v}_\perp, \mathbf{u}_\perp) = \int_\Omega \mathbf{v}_\perp \cdot \mathbf{u}_\perp d\Omega$ and also $(\mathrm{v}_z, \mathrm{u}_z) = \int_\Omega \mathrm{v}_z \mathrm{u}_z d\Omega$.

Edge element discretization.

In this approach we set up a direct discrete analog to problem (5) and additional to the divergence condition (4). The weak form of the waveguide eigenvalue problem is to find k_z, $\mathbf{u}_\perp$, u_z, such that for any $\mathbf{v}_\perp \in \mathrm{H}_0(\mathrm{curl}, \Omega)$ and $\mathrm{v}_z \in \mathrm{H}_0^1(\Omega)$

$$\begin{aligned}
\left(\nabla_\perp \times \mathbf{v}_\perp, \epsilon_r^{-1} \nabla_\perp \times \mathbf{u}_\perp\right) + k_z \cdot \left(\mathbf{v}_\perp, \epsilon_r^{-1} \nabla_\perp \mathrm{u}_z\right) & & \\
+k_z^2 \cdot \left(\mathbf{v}_\perp, \epsilon_r^{-1} \mathbf{u}_\perp\right) &= +k_0^2 \cdot (\mathbf{v}_\perp, \mathbf{u}_\perp) & (7)\\
\left(\nabla_\perp \mathrm{v}_z, \epsilon_r^{-1} \nabla_\perp \mathrm{u}_z\right) + k_z \cdot \left(\nabla_\perp \mathrm{v}_z, \epsilon_r^{-1} \mathbf{u}_\perp\right) &= k_0^2 \cdot (\mathrm{v}_z, \mathrm{u}_z) & (8)\\
(\nabla_\perp \mathrm{v}_z, \mathbf{u}_\perp) &= k_z \cdot (\mathrm{v}_z, \mathrm{u}_z)\,. & (9)
\end{aligned}$$

In order to derive these equations, we use the continuity of $\mathrm{E}_z = \epsilon_r^{-1} \nabla_\perp \times \mathbf{u}_\perp$, so that all line integrals over Γ_{ij} and Γ_{ji} cancel in the interior of Ω.
It is an important fact that a solution $(\mathbf{u}_\perp, \mathrm{u}_z) \in \mathrm{H}_0(\mathrm{curl}, \Omega) \times \mathrm{H}_0^1(\Omega)$ of the equations (7), (8) with finite k_z and k_0 also satisfies the divergence condition (9). This can be seen by the special choice $\mathbf{v}_\perp = -1/k_z \cdot \nabla_\perp \mathrm{v}_z \in \mathrm{H}_0(\mathrm{curl}, \Omega)$ and inserting equation (8) into (7).
Given a regular triangulation of Ω, the structure of (7)-(9) can be passed on to a discrete version by using edge elements ([16],[4], [1]) for the transversal components and nodal elements for u_z . Let $\mathrm{V}_\perp \subset \mathrm{H}_0(\mathrm{curl}, \Omega)$, $\mathrm{V}_z \subset \mathrm{H}_0^1(\Omega)$ be the corresponding linear finite element spaces with bases $\psi_1 \cdots \psi_m$ and $\phi_1 \cdots \phi_p$.

Here m is the number of interior edges and p is the number of inner points of the triangulation. We introduce the system matrices

$$
\begin{array}{rclrcl}
(\mathrm{A}_\perp)_{jk} & = & \left(\nabla_\perp \times \psi_j, \epsilon_r^{-1} \nabla_\perp \times \psi_k\right), & (\mathrm{A}_z)_{jk} & = & \left(\nabla_\perp \phi_j, \epsilon_r^{-1} \nabla_\perp \phi_k\right), \\
(\mathrm{B}_\perp)_{jk} & = & \left(\psi_j, \epsilon_r^{-1} \psi_k\right), & (\mathrm{M}_z)_{jk} & = & (\phi_j, \phi_k) \\
(\mathrm{M}_\perp)_{jk} & = & (\psi_j, \psi_k).
\end{array}
\tag{10}
$$

The weak gradient of ϕ_j is an element of $\mathrm{V}_\perp$, so we may define G to be the matrix representation (for the above bases) of the linear map

$$
\nabla_\perp : \mathrm{V}_z \longrightarrow \mathrm{V}_\perp.
$$

In this way we arrive at the discretized version of (7)-(8)

$$
\underbrace{\begin{bmatrix} \mathrm{A}_\perp + k_z^2 \cdot \mathrm{B}_\perp & k_z \cdot \mathrm{B}_\perp \mathrm{G} \\ k_z \cdot \mathrm{G}^* \mathrm{B}_\perp & \mathrm{A}_z \end{bmatrix}}_{\mathrm{A}_{\mathrm{res}}} \begin{bmatrix} \mathrm{u}_\perp \\ \tilde{\mathrm{u}}_z \end{bmatrix} = k_0^2 \cdot \underbrace{\begin{bmatrix} \mathrm{M}_\perp & 0 \\ 0 & \mathrm{M}_z \end{bmatrix}}_{\mathrm{M}_{\mathrm{res}}} \begin{bmatrix} \mathrm{u}_\perp \\ \tilde{\mathrm{u}}_z \end{bmatrix}, \tag{11}
$$

and the discrete divergence condition

$$
\begin{bmatrix} \mathrm{G} \\ -\mathrm{I} \end{bmatrix}^* \begin{bmatrix} \mathrm{M}_\perp & 0 \\ 0 & k_z \cdot \mathrm{M}_z \end{bmatrix} \begin{bmatrix} \mathrm{u}_\perp \\ \mathrm{u}_z \end{bmatrix} = 0. \tag{12}
$$

As in the continuous system, the divergence condition (12) automatically holds for a solution $(\mathbf{u}_\perp, \mathrm{u}_z)$ of (13) with finite k_z and k_0. Problem (11) is a standard eigenvalue problem $\mathrm{A}_{\mathrm{res}} u = \lambda \mathrm{M}_{\mathrm{res}} u$ for $\lambda = k_0^2$ with a selfadjoint matrix $\mathrm{A}_{\mathrm{res}}$ and a positive definite mass matrix $\mathrm{M}_{\mathrm{res}}$. Here the unknown propagation constant k_z appears implicitly. As above for the continuous problem, we may rearrange equation (11) by substituting $\tilde{\mathrm{u}}_z = k_z \cdot \mathrm{u}_z$ we arrive at an explicit eigenvalue problem

$$
\underbrace{\left(\begin{bmatrix} \mathrm{A}_\perp & \mathrm{B}_\perp \mathrm{G} \\ 0 & \mathrm{A}_z \end{bmatrix} - k_0^2 \cdot \begin{bmatrix} \mathrm{M}_\perp & 0 \\ 0 & \mathrm{M}_z \end{bmatrix} \right)}_{\mathrm{A}} \begin{bmatrix} \mathrm{u}_\perp \\ \mathrm{u}_z \end{bmatrix} = -k_z^2 \cdot \underbrace{\begin{bmatrix} \mathrm{B}_\perp & 0 \\ \mathrm{G}^* \mathrm{B}_\perp & 0 \end{bmatrix}}_{\mathrm{B}} \begin{bmatrix} \mathrm{u}_\perp \\ \mathrm{u}_z \end{bmatrix} \tag{13}
$$

for k_z. Since the above matrix B is singular, this formulation is not well suited for the construction of a multigrid method. That is why, in the following, we will focus on a multigrid algorithm for equation (11), which we will solve for k_z, subject to the divergence condition (12).

Nodal element discretization.

We use the divergence condition (4) to substitute H_z in (2), which gives the modified transversal equation [10]

$$
\nabla_\perp \times \epsilon_r^{-1} \nabla_\perp \times \mathbf{u}_\perp - \epsilon_r^{-1} \nabla_\perp (\nabla_\perp \cdot \mathbf{u}_\perp) - k_0^2 \mathbf{u}_\perp = -k_z^2 \epsilon^{-1} \mathbf{u}_\perp, \tag{14}
$$

where only the transverse field $\mathbf{u}_\perp$is involved. The corresponding weak problem now reads

$$\begin{aligned} \left(\nabla_\perp \times \mathbf{v}_\perp, \epsilon_r^{-1}\nabla_\perp \times \mathbf{u}_\perp\right) - k_0^2 \cdot (\mathbf{v}_\perp, \mathbf{u}_\perp) &\quad + \\ \textstyle\sum_{i=1}^N \int_{\Omega_i} (\nabla_\perp \cdot \epsilon_r^{-1}\mathbf{v}_\perp)(\nabla_\perp \cdot \mathbf{u}_\perp) d\Omega_i &\quad + \\ -\textstyle\sum_{i,j=1}^N \int_{\Gamma_{ij}} (\mathbf{n}\cdot\mathbf{v}_\perp)\epsilon_r^{-1}(\nabla_\perp \cdot \mathbf{u}_\perp) ds &\quad = \\ -k_z^2 \cdot \left(\mathbf{v}_\perp, \epsilon_r^{-1} \cdot \mathbf{u}_\perp\right) & \end{aligned} \tag{15}$$

for all $\mathbf{v}_\perp \in \mathrm{H}_0^1(\Omega) \times \mathrm{H}_0^1(\Omega)$.
As above all line integrals involving $\mathrm{E}_z = \epsilon^{-1}\nabla_\perp \times \mathbf{u}_\perp$ vanish in the interior of Ω. This is not the case for the second sum in (15), because $\nabla_\perp \cdot \mathbf{u}_\perp = ik_z\mathrm{H}_z$ is continuous and hence $\epsilon_r^{-1}\nabla_\perp \cdot \mathbf{u}_\perp$ may jump across Γ_{ij}. In (15) not only the curl - operator but also the div - operator act on $\mathbf{u}_\perp$, which inhibits the use of linear edge elements for the transversal field. A finite element discretization based on the linear nodal elements space $\mathrm{V}_\perp \subset \mathrm{H}_0^1(\Omega) \times \mathrm{H}_0^1(\Omega)$ is yielding straightforward the algebraic system

$$\mathrm{Au}_\perp = -k_z^2 \cdot \mathrm{Mu}_\perp, \tag{16}$$

with a non-symmetric matrix A and a canonical mass matrix M.

3 Multigrid algorithms

In an adaptive finite element discretization of the above problems we have a set of sequentially refined triangulations $\{\mathcal{T}_h\}$ of Ω with corresponding finite element spaces $\mathrm{V}_h \subset \mathrm{H}_0(\mathrm{curl}, \Omega) \times \mathrm{H}_0^1(\Omega)$ resp. $\mathrm{V}_h \subset \mathrm{H}_0^1(\Omega) \times \mathrm{H}_0^1(\Omega)$. In each case this yields an algebraic eigenvalue problem $\mathrm{A}_h\mathrm{u} = \lambda \cdot \mathrm{B}_h\mathrm{u}$. As in [12][13] we generalize this problem for the ability to calculate simultaneously a certain number q of clustered or degenerate eigenvalues with smallest real part. Hence we seek a q - dimensional invariant subspace U_h, in particular

$$\mathrm{A}_h\mathrm{U}_h = \mathrm{B}_h\mathrm{U}_h\mathrm{T}_h. \tag{17}$$

As mentioned above the structure of equation (17) depends on the chosen discretization. The edge element discretization for the waveguide problem (13) leads to a singular matrix B_h, whereas a nodal basis discretization of the modified transversal equation (14) and the resonance problem (11) give a canonical mass matrix B_h. There exist different multigrid solvers for the above problem with a positive definite B [14], [5], [6]. Here we present the method developed in [12] for the Helmholtz eigenvalue problem. The formulation of the waveguide problem based on the modified transversal equation fits perfectly into this multigrid concept. Therefore we can extend this algorithm directly to the vectorial case. Unfortunately, this is not true for magnetic or lossy materials. In these cases the mass matrix B_h is no longer positive definite.

3.1 General concept

In the following we suppress the subindex h and assume B to be a positive definite operator. The backbone of our method is a pcg-like iterative eigenvalue

solver for problem (17), see [11]. The main advantage of this method is that it allows the handling of subspaces whose B - orthonormality will not be destroyed by the algorithm. As in [12] we use this method as a *smoother.* This method reduces the high-frequency error on each grid very effectively and gets inefficient after a few iterations. How does the smoother works ?
Recall that the above eigenvalue problem admits a Schur decomposition

$$\mathrm{AQ} = \mathrm{BQK}, \quad \mathrm{Q}^{'}\mathrm{BQ} = \mathrm{Id}.$$

Herein $\mathrm{K} = \mathrm{diag}\,(\mathrm{K}_i)$ is a block diagonal matrix, with upper triangular blocks K_i. To each K_i corresponds an invariant subspace $\mathrm{E_i}$. The subspaces $\mathrm{E_i}$ are chosen so that they possess no non-trivial invariant subspace. The matrices $\mathrm{K_i}$ depend on the chosen B - orthonormal basis, while $\mathrm{trace}\,\mathrm{K_i}$ does not depend on it. Any q-dimensional invariant subspace Y is the sum of particular $\mathrm{E_i}$, say

$$\mathrm{Y} = \mathrm{E}_{\mathrm{i}_1} + \cdots + \mathrm{E}_{\mathrm{i}_{\mathrm{n_Y}}}.$$

To Y corresponds the upper triangular matrix $\mathrm{Z} = \mathrm{diag}_{l=1\ldots n_{\mathrm{Y}}}\,(\mathrm{K}_{i_l})$. Hence we may define $\mathrm{trace}\,\mathrm{Y} = \mathrm{trace}\,\mathrm{Z}$. We characterize the sought q-dimensional invariant subspace U with corresponding upper triangular matrix T by

$$\mathrm{trace}\,\mathrm{U} = \min\,\{\mathrm{trace}\,\mathrm{Y} \mid \mathrm{Y} \text{ is } q\text{-dimensional invariant subspace}\}$$

Details of this algorithm are given in Algorithm 1.

Algorithm 1 Döhler pcg as smoother with ν iteration steps

Require: $\mathrm{U}^{(0)}, \mathrm{T}^{(0)}$ {initial guess}
  $\mathrm{G} = \mathrm{C}^{-1}\left(\mathrm{AU}^{(0)} - \mathrm{BU}^{(0)}\mathrm{T}^{(0)}\right)$
  $\mathrm{P} = \mathrm{G}$ {initial correction space}
  for $k = 0$ to ν **do**

$$\left.\begin{array}{lcl} \tilde{\mathrm{A}} & = & \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right]^{'} \mathrm{A} \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right] \\ \tilde{\mathrm{B}} & = & \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right]^{'} \mathrm{B} \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right] \end{array}\right. \{\text{projected problem}\}$$

$$\left.\begin{array}{lcl} \left[\begin{array}{cc} \tilde{\mathrm{U}} & \tilde{\mathrm{S}} \end{array}\right]^{'} \tilde{\mathrm{A}} \left[\begin{array}{cc} \tilde{\mathrm{U}} & \tilde{\mathrm{S}} \end{array}\right] & = & \begin{pmatrix} \mathrm{T}^{(k)} & 0 \\ 0 & \mathrm{T_S} \end{pmatrix} \\ \left[\begin{array}{cc} \tilde{\mathrm{U}} & \tilde{\mathrm{S}} \end{array}\right]^{'} \tilde{\mathrm{B}} \left[\begin{array}{cc} \tilde{\mathrm{U}} & \tilde{\mathrm{S}} \end{array}\right] & = & \mathrm{Id} \end{array}\right. \{\text{Schur decomposition}\}$$

  $\mathrm{U}^{(k+1)} = \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right] \tilde{\mathrm{U}}$ {update of U}
  $\mathrm{S} = \left[\begin{array}{cc} \mathrm{U}^{(k)} & \mathrm{P} \end{array}\right] \tilde{\mathrm{S}}$
  $\mathrm{G} = \mathrm{C}^{-1}\left(\mathrm{AU}^{(k)} - \mathrm{BU}^{(k)}\mathrm{T}^{(k)}\right)$

  solve for X : $\quad \mathrm{T_S X} - \mathrm{XT}^{(k)} = -\mathrm{P}^{'}\left(\mathrm{AG} - \mathrm{BGT}^{(k)}\right)$ {Sylvester equation}
  $\mathrm{P} = \mathrm{G} + \mathrm{SX}$ {new correction space}
  end for

Given an initial guess $\mathrm{U}^{(0)}, \mathrm{T}^{(0)}$ for the sought q - dimensional invariant subspace on the finest grid we construct a *correction space* P in a pcg-like manner. We use for example a Jacobi iteration step as the preconditioning matrix C^{-1}. Now, we correct $\mathrm{U}^{(0)}$ by solving a small projected eigenvalue problem (*Ritz step).* Assuming that the q smallest eigenvalues are sufficiently well approximated such that there is a spectral gap between the q first eigenvalues and the remaining ones of the projected system, the Schur decomposition in Algorithm 1 supplies upper triangular matrices $\mathrm{T}^{(\mathrm{k})} \in \mathbb{C}^{q\times q}$, $\mathrm{T_S} \in \mathbb{C}^{q\times q}$ with

$$\mathrm{Re}(\mathrm{T}_{11}^{(k)}) \leq \cdots \leq \mathrm{Re}(\mathrm{T}_{qq}^{(k)}) \leq \mathrm{Re}(\mathrm{T}_{\mathrm{S},11}) \leq \cdots \leq \mathrm{Re}(\mathrm{T}_{\mathrm{S},qq}).$$

This correction procedure is motivated by the minimal principle above. After the correction of U we have to construct a new correction space P which is done similar to the pcg-method again.
The proposed correction space P in Algorithm 1 is generated by a multiplication of the current U with the discrete second order "differential operator" $(\mathrm{A}[\cdot] - \mathrm{B}[\cdot]\,\mathrm{T})$ and hence high-frequency errors are overstressed in P. But fortunately, by the multigrid structure we can force low-frequency corrections to appear in P. So, given the prolongation matrix I_H^h from any coarse grid to the current fine grid, we restrict the eigenvalue problem to the subspace $\left[\begin{array}{cc} \mathrm{U} & \mathrm{I}_H^h \end{array}\right]$, especially

$$\underbrace{\left[\begin{array}{cc} \mathrm{U} & \mathrm{I}_H^h \end{array}\right]^{'} \mathrm{A} \left[\begin{array}{cc} \mathrm{U} & \mathrm{I}_H^h \end{array}\right]}_{\tilde{\mathrm{A}}} \tilde{\mathrm{U}} = \underbrace{\left[\begin{array}{cc} \mathrm{U} & \mathrm{I}_H^h \end{array}\right]^{'} \mathrm{B} \left[\begin{array}{cc} \mathrm{U} & \mathrm{I}_H^h \end{array}\right]}_{\tilde{\mathrm{B}}} \tilde{\mathrm{U}}\mathrm{T} \qquad (18)$$

and carry out Algorithm 1 for this restricted problem. Alternatively, this procedure may be interpreted in the sense that we just use the coarse grid basis I_H^h to construct low-frequency correction spaces P (see Algorithm 1).
On the coarsest level we may use an exact solver or the iterative method (1) with a fixed number of iterations as well.

3.2 Edge element method for waveguide problem

Algorithm 1 is based on the Schur decomposition of a small restricted eigenvalue problem which can only be done if B_h is a positive definite matrix. But this is not the case in our variational formulation (13). Therefore we go one step back to equation (5) and its discrete analog (11) in which the desired value k_z appears implicitly within the selfadjoint eigenvalue problem $\mathrm{A}_{\mathrm{res}}(k_z)\mathrm{u} = k_0^2\mathrm{M}_{\mathrm{res}}\mathrm{u}$. The idea now is to solve this equation for k_z by a Newton-like iteration. To keep the notation simple, we outline this algorithm for the case of a single non-degenerate eigenvalue k_z in the self-adjoint case ($q = 1$). Assume that we can solve $\mathrm{A}_{\mathrm{res}}(k_z)\mathrm{u} = (k_0^2 + \delta)\cdot \mathrm{M}_{\mathrm{res}}\mathrm{u}$ in a neighborhood of the exact value for k_z and that the "disturbed" normalized eigenvector $\mathrm{u} = \mathrm{u}(k_z)$ depends smoothly on k_z. The disturbed resonance wave number is given by the Rayleigh quotient

$$\left(k_0^2 + \delta\right) = \frac{\mathrm{u}^{\mathrm{T}}\mathrm{A}_{\mathrm{res}}(k_z)\mathrm{u}}{\mathrm{u}^{\mathrm{T}}\mathrm{M}_{\mathrm{res}}\mathrm{u}}$$

and k_z is determined via the condition $\delta(k_z) = 0$. On the basis of

$$\delta^{'}(k_z) = \mathrm{u}^{\mathrm{T}}(k_z)\mathrm{A}_{\mathrm{res}}^{'}(k_z)\mathrm{u}(k_z) + \underbrace{\mathrm{u}^{\mathrm{T}}(k_z)\mathrm{A}_{\mathrm{res}}(k_z)\mathrm{u}^{'}(k_z)}_{\mathcal{O}(\delta)},$$

we may construct a *Newtion-like iteration* dropping the $\mathcal{O}(\delta)$-thus arriving at the iteration

$$k_z^{(i+1)} = k_z^{(i)} - \frac{\delta(k_z^{(i)})}{\mathrm{u}^{\mathrm{T}}(k_z^{(i)})\mathrm{A}'_{\mathrm{res}}(k_z^{(i)})\mathrm{u}(k_z^{(i)})},$$

The convergence properties of such an iteration are roughly the same as for a simplified Newton iteration [9, chapter 2]. Numerical tests also show, that this Newton-like iteration converges very fast, if we use the k_z obtained from the coarser grid as the initial guess. In order to get an algorithm of multigrid complexity we need a multigrid solver for the resonance problem $\mathrm{A}_{\mathrm{res}}(k_z)\mathrm{u} = (k_0^2 + \delta) \cdot \mathrm{M}_{\mathrm{res}}\mathrm{u}$.

3.3 Edge element method for resonance problem

Even the selfadjoint resonance problem (11) fits well into our multigrid concept, some difficulties may arise due to the null space of the operator $\mathrm{A}_{\mathrm{res}}$ and to the fact that we are only interested in positive eigenvalues close to k_0^2. Therefore a method which minimizes the Rayleigh quotient will converge to this null space. As can be seen in equation (5), the null space consists in the continuous case of 3D-curl-free vector fields

$$\begin{bmatrix} \nabla_\perp \varphi \\ -ik_z\varphi \end{bmatrix}.$$

This null space is closely tied to the divergence condition (4), see [3]. In fact, by solving the Poisson problem

$$-\Delta_\perp \varphi + k_z^2\varphi = (ik_z\mathrm{H}_z - \nabla_\perp \cdot \mathbf{H}_\perp),$$

one can split the magnetic field into 3D-div-free and curl-free parts (Helmholtz decomposition)

$$\begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{H}_z \end{bmatrix} = \underbrace{\begin{bmatrix} \nabla_\perp \varphi \\ -ik_z\varphi \end{bmatrix}}_{\mathrm{curl-free}} + \underbrace{\begin{bmatrix} \mathbf{H}_\perp \\ \mathrm{H}_z \end{bmatrix}}_{\mathrm{div-free}}.$$

The curl-free part is non-physical and violates the divergence condition. Following [15], [2, p. 122] we remove that part throughout the multigrid algorithm, whenever it arises (projection to the div-free subspace).

4 Numerical examples

The above two algorithms have been implemented in our fully adaptive software package ModeLab. In order to compare the nodal with the edge element discretization on the same hierarchy of grids we restrict ourselves to uniform mesh refinements for the following problems. In each problem choose $k_0 = 2\pi/1.55$ and the smallest eigenvalue is computed ($q = 1$). Recall, that the refractive of an material is defined via $n^2 = \epsilon_r$. In case of the edge element discretization we solve for k_z by a Newton iteration. In each Newton step we solve a resonance problem by our multigrid algorithm. In the Tables 1-3 we give the required cycles per Newton step to reduce the error to a relative residual of 10^{-5}.

Table 1: *Rectangular core waveguide.* Required cycles of our multigrid-method and approximated eigenvalue on each level and Newton iteration. The relative residual error is reduced to 10^{-5}.

	edge		nodal	
Level	cycles	k_z	cycles	k_z
1	-	2.5558	-	2.5362
2	3+1	2.5555	3	2.5474
3	3+1	2.5554	3	2.5518
4	2+0	2.5554	3	2.5537

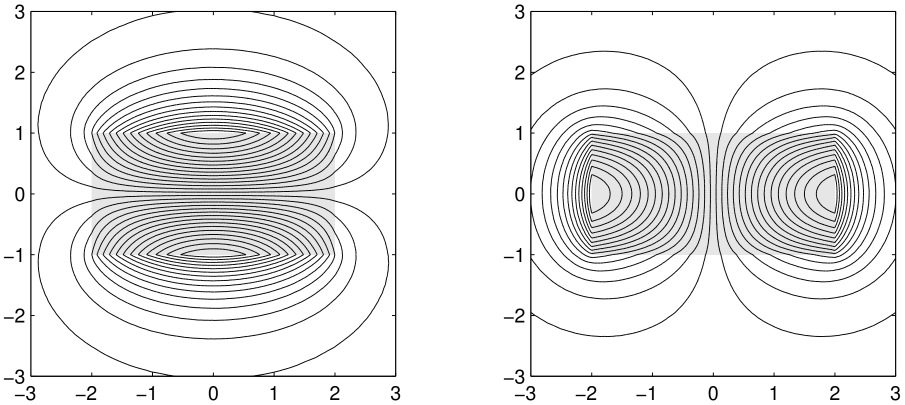

Figure 3: *Rectangular core waveguide.* Isolines of the H_z-components computed with the edge element discretization. The rectangular core is plotted in grey.

Rectangular core Waveguide.

The geometry consists of a rectangular core of relative size $1:2$ and $n = 0.7$ embedded in a medium with $n_{\text{medium}} = 0.5$. As can be seen in Table 1, the approximation of the eigenvalue k_z is much better in the edge element discretization. In this example the Maxwell solution differs significantly from the Helmholtz approximation, which provides $k_z = 2.5724$. In Fig. 3 the H_z-components of the two orthogonal eigenfunctions of smallest eigenvalue are plotted. In the Helmholtz approximation these components are assumed to be zero.

Rib waveguide.

The geometry is sketched in Fig. 2. Outside the waveguide we have a medium of $n = 1$.The relative permittivity of the horizontal stripe with a width of 0.2 is $n = 3.38$. This strip is embedded in a material of permittivity $n = 3.17$ at distance 0.2 to the medium. The rectangular rib has a size of 2.4×1. Again, the edge element discretization approximates the eigenvalues far better than the nodal one (Table 2). Furthermore the number of cycles diminishes in each step for the edge element discretization. The magnetic field strength is plotted in Fig. 4. You can see a singularity-like H_z-distribution at the corner of the ribs.

Table 2: *Rib waveguide* (compare Table 1).

	edge		nodal	
Level	cycles	k_z	cycles	k_z
1	-	12.9685	-	12.9572
2	19+2	12.9672	6	12.9624
3	9+0	12.9669	12	12.9647
4	6+0	12.9668	10	12.9658

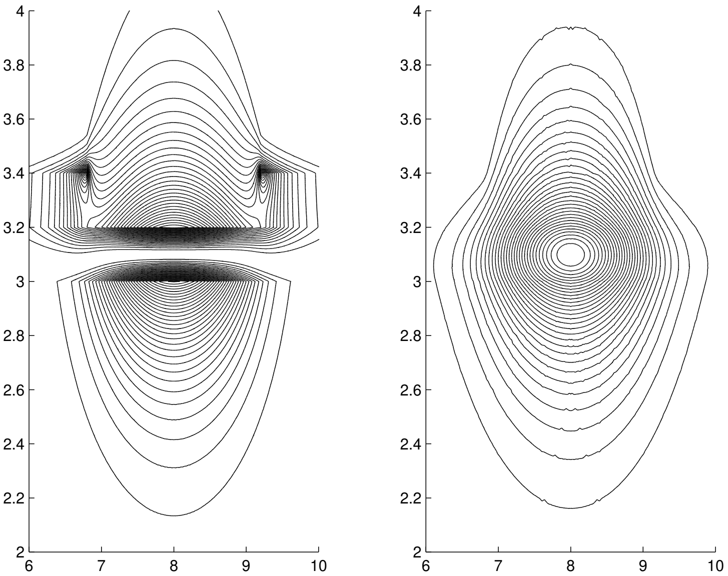

Figure 4: *Rib waveguide.* Isolines of H_z^2 (left) and $\mathrm{H}_\perp^2$ (right).

Table 3: *Circular optical fiber* (compare Table 1).

Level	edge cycles	edge k_z	nodal cycles	nodal k_z
1	-	6.1308	-	6.1295
2	3+1	6.1317	2	6.1307
3	3+0	6.1313	2	6.1310
4	2+0	6.1313	2	6.1311

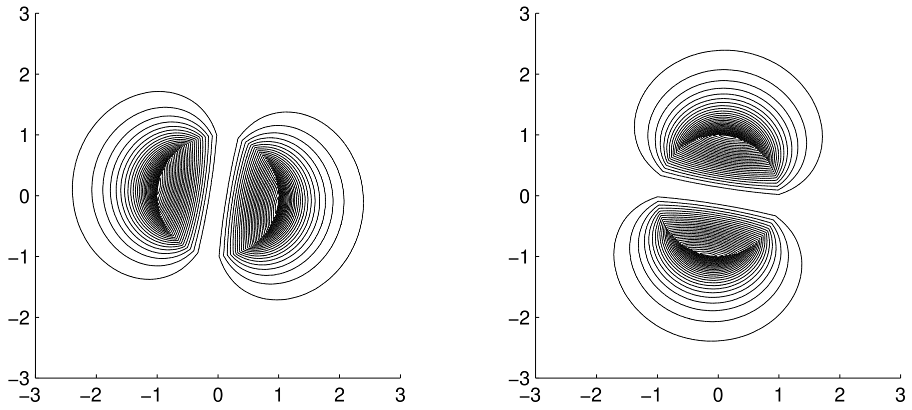

Figure 5: Circular optical fiber. Isolines of H_z^2 of two orthogonal eigenfunctions.

Circular optical fiber.

The optical fiber consists of a circular core with diameter 2 and permittivity $n = 1.55$ embedded in a medium of permittivity $n_{\mathrm{medium}} = 1.5$. Due to rotational symmetry the lowest eigenvalue is twice degenerated. As can be seen in Table 3 both variants converge after a small number of cycles per level. As in the above two examples the edge element discretization approximates the eigenvalue better. In Fig. 5 we plot the H_z-components of two orthogonal eigenfunctions.

5 Conclusions

The multigrid concept developed earlier for the scalar Helmholtz equation has been extended herein to vectorial time-harmonic Maxwell's equations in non-magnetic materials. The algorithm depends on the chosen finite element discretization of the magnetic field. Using the divergence condition one can eliminate the H_z-component, which leads to a modified transversal Maxwell equation, which may be discretized by nodal elements. Alternatively, we have directly discretized Maxwell's equations by linear edge elements for the transversal components and nodal elements for the H_z-component thus setting up a discrete analog of the continuous Maxwell equations. For both variants a multigrid algorithm has been presented. It is shown experimentally that the edge element discretization approximates the eigenvalues clearly better already on rather coarse grids. All our codes are collected in the software package ModeLab, which also includes adaptive mesh refinements.

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