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On the Computation of Eigenmodes of Integrated Optical Components

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Abstract

The paper deals with the solution of the eigenvalue problem of the complex Helmholtz equation. We concentrate on multigrid methods for solving the algebraic eigenproblems arising from discretization with finite elements by using adaptive generated meshes. An illustrative numerical example, the simulation of a waveguide structure from integrated optics, is included.

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1 Introduction

Optical fibers are important components of modern telecommunication. In particular, almost all communication networks are based on optical fiber techniques. The advantages of optical versus electrical signal transmission are the larger bandwidth and the lower transmission losses.

In the early seventies, the idea was born to combine this optical signal transmission with optical signal processing. The aim was to build integrated optical chips consisting of active and passive components analogously to semiconductor chips. The realization of this concept was inhibited by considerable technological difficulties arising in the manufacturing of such optical devices. However, significant technical problems could be solved in the last ten years and the idea of integrated optical chips has undergone a revival.

Apart from the solution of the technological problems, the development of appropriate physical models and the numerical simulation of optical components have been central research topics. In principle, it is desired to carry out the complete design of an optical chip with one simulation tool. Since this problem has an enormous complexity, the most popular approach to simulate the behaviour of optical chips is to separately investigate particular optical components like waveguides, couplers, or lasers. A decisive prerequisite for the design of such components is the knowledge of their eigenmodes.

The subject of this paper is twofold. First, we present the scalar complex Helmholtz equation as a commonly used mathematical model for the simulation of optical devices. Since the interesting components are invariant in one direction, the computation of modes, which propagate in this direction, leads in a natural way to the eigenvalue problem of the Helmholtz equation in two space dimensions. This eigenproblem can be both selfadjoint, in case of loss free propagation, and nonselfadjoint, in case of damped or amplified propagation. Secondly we discuss multigrid algorithms for the solution of the selfadjoint as well as the nonselfadjoint eigenproblem. The discretization by finite elements is the starting point of our considerations.

Typically, the computation of modes of integrated optical devices is characterized by the following difficulties: At first, the components possess a multiscale structure with scale ratios up to one to one thousand. Next, large and abrupt jumps occur in the material parameters. As mentioned above, the eigenvalue problem may be nonselfadjoint. And last, clusters of neighbouring eigenvalues must be resolved, often with a high accuracy. The consequences for the treatment of the described problem class are, on one hand, the use of adaptive meshes for discretization of the continuous problem and, on the other hand, the use of simultaneous eigenproblem solvers for the solution of the discrete problems.

2 The Problem

The propagation of light in optical components is described by the time harmonic Maxwell equations for the electrical and magnetical fields \mathbf{E} and \mathbf{H} in isotropic, nonmagnetic, and sourceless media

$$\begin{aligned} \text{curl } \mathbf{H} &= (i\omega\epsilon + \sigma) \mathbf{E}, & \text{div } \mathbf{H} &= 0, \\ \text{curl } \mathbf{E} &= -i\omega\mu \mathbf{H}, & \text{div } \epsilon\mathbf{E} &= 0 \end{aligned}$$

with permittivity ϵ , permeability μ , conductivity σ , and optical angular frequency ω . If we take the curl of the first equation, we see by use of the third equation and by introducing the complex permittivity $\tilde{\epsilon} = \epsilon - i\sigma/\omega$, that the magnetic field satisfies the vector wave equation

$$\text{curl } \frac{1}{\tilde{\epsilon}} \text{curl } \mathbf{H} = \omega^2 \mu \mathbf{H} \quad .$$

This equation transforms into

$$-\Delta \mathbf{H} - \omega^2 \tilde{\epsilon} \mu \mathbf{H} = \nabla \log \tilde{\epsilon} \times \text{curl } \mathbf{H} \quad (1)$$

by employing the rules of vector calculus and the divergence-free condition for \mathbf{H} . However, for the simulation of most optical components, a simplified model is adequate [18]. We neglect the coupling term on the right hand side of (1) and obtain the vector Helmholtz equation

$$-\Delta \mathbf{H} - \omega^2 \tilde{\epsilon} \mu \mathbf{H} = 0 \quad .$$

In cartesian coordinates the vector Laplace operator simplifies to the usual scalar one, applied to each component of the field vector independently. Thus we do not need to distinguish between the vector components of \mathbf{H} , and it is sufficient to consider the scalar Helmholtz equation

$$-\Delta H - \omega^2 \tilde{\epsilon} \mu H = 0 \quad , \quad (2)$$

where H is any component of the magnetic field \mathbf{H} . We use equation (2) as a scalar approximation of the field description given by the full Maxwell equations.

A characteristic feature of the interesting optical structures is its invariance in one direction. As an example, a typical component, the waveguide, is represented in Figure 1. In the following we assume that this particular direction is the z -direction. Since we want to compute modes which propagates in this

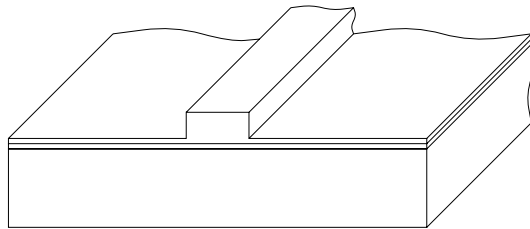


Figure 1: A typical integrated optical component: waveguide.

direction, the component H of the magnetic field has to obey the separation ansatz

$$H(x, y, z) = u(x, y) e^{-ikz}$$

in terms of the amplitude function $u(x, y)$ and the wave number k in z -direction. The real part of k gives the phase velocity, the imaginary part of k gives information about damping or amplification in z -direction. If we insert the separation ansatz into equation (2), we obtain the eigenproblem of the scalar Helmholtz equation

$$-\Delta u - \omega^2 \tilde{\epsilon} \mu u = -k^2 u \quad . \quad (3)$$

Since the components of the magnetic field of the interesting modes are restricted to a small region of the plane, we consider problem (3) only in a bounded two dimensional subset Ω , equipped with Dirichlet boundary condition. Hence, the complete model for integrated optical components is given by

$$\begin{aligned} -\Delta u(x, y) - f(x, y) u(x, y) &= \lambda u(x, y), & (x, y) \in \Omega \\ u(x, y) &= 0, & (x, y) \in \partial\Omega \quad , \end{aligned} \quad (4)$$

where $f(x, y) = \omega^2 \tilde{\epsilon}(x, y, \omega) \mu$ and $\lambda = -k^2$. In media with electrical conductivity, the permittivity $\tilde{\epsilon}$, and hence the function f , is complex valued. Therefore, in general, the eigenvalues λ and the eigenfunctions u may be complex valued.

3 Multigrid Algorithms for Eigenproblems

In the context of finite element methods, it is standard to consider the eigenvalue problem (4) in its variational form: determine weak eigenfunctions

$u \in H_0^1(\Omega) \setminus \{0\}$ and eigenvalues $\lambda \in \mathbb{C}$ such that

$$a(v, u) = \lambda (v, u) \quad \forall v \in H_0^1(\Omega) \quad . \quad (5)$$

The sesquilinear form $a(\cdot, \cdot)$ is defined by

$$a(v, u) = (\nabla v, \nabla u) - (v, f u) \quad ,$$

the inner product (\cdot, \cdot) is the usual $L^2(\Omega)$ scalar product. We assume that Ω is an open, bounded, and connected subset of \mathbb{R}^2 , and $f \in L^\infty(\Omega)$.

In our problem class only the eigenfunctions corresponding to the eigenvalues with lowest real parts are of interest. Both from the theoretical and the numerical point of view it is appropriate to consider the eigenproblem in a modified formulation. A perturbation analysis, as in the case of matrices, shows, that the sensitivity of the eigenfunctions with respect to perturbations in f depends on the spectral gap of the interesting eigenvalues from the remaining part of the spectrum. We can conclude, that the invariant subspace spanned by sensitive eigenfunctions may be insensitive, if the corresponding eigenvalues are sufficiently separated from the rest of the spectrum. Hence, instead of (5), we will consider the eigenproblem in the context of invariant subspace computations, i. e., in the following form: determine functions $u_j \in H_0^1(\Omega) \setminus \{0\}$ and values $\tau_{kj} \in \mathbb{C}$ satisfying

$$a(v, u_j) = \sum_{k=1}^j \tau_{kj} (v, u_k) \quad \forall v \in H_0^1(\Omega) \quad , \quad (6)$$

where $(u_k, u_j) = \delta_{kj}$, $\tau_{jj} = \lambda_j$ and $j = 1, \dots, q$ (q is the number of desired eigenvalues with lowest real parts). The special form (6) is the continuous analogue to the partial Schur decomposition of a matrix [11]. The functions u_j are referred as Schur functions. In the special case of a selfadjoint eigenvalue problem, i. e., of a real valued function f , the values τ_{kj} with $k < j$ vanish, i. e., the functions u_j are eigenfunctions.

The discretization of (6) by finite elements leads to the generalized matrix Schur problem

$$AU = BUT, \quad U^*BU = I \quad . \quad (7)$$

The system matrix A and the mass matrix B are sparse $(N \times N)$ -matrices, where N is the dimension of the underlying finite element space. The matrix B is the Gram matrix of the basis functions of the finite element space, and hence, by definition, selfadjoint and positive definite. The unknown matrix U is a full $(N \times q)$ -matrix consisting of the coefficients of the discrete Schur

functions with respect to the finite element basis functions, whereas the unknown matrix T is an upper triangular $(q \times q)$ -matrix formed by approximate values τ_{kj} . The value N lies typically between 10^3 and 10^5 , the number q ranges from 1 to 10. Hence, we have to determine a low-dimensional invariant subspace of a large sparse matrix pencil.

There exists many numerical algorithms to solve the discrete eigenproblem (7), see, e. g., the recent survey article by van der Vorst and Golub [21], where the emphasis lies on Krylov subspace methods. Here, we focus on multigrid algorithms. A characteristic feature of these methods is their optimal complexity, i. e., the effort for the solution of (7) is proportional to the number N of degrees of freedom. Hence, multigrid methods are very effective, especially in the context of problems with a large number of unknowns. Any of these methods needs a hierarchy of discretization meshes. In view of the difficulties arising in our problem class, we construct this sequence by adaptive mesh refinement. We will restrict ourselves to conforming methods, i. e., the corresponding finite element spaces satisfy the relation

$$V_0 \subset V_1 \subset \dots \subset V_{l_{\max}} \subset H_0^1(\Omega) .$$

First we describe the principle of these methods for the special two grid case. Every iteration step of the method is divided in two stages, the smoothing step and the coarse grid correction step. In the smoothing step on the fine grid, a simple iteration method (the smoother) damps the error components corresponding to high frequencies. Then, a coarse grid correction problem (of significant smaller dimension as the original problem) is solved to handle the error components corresponding to low frequencies. By alternating smoothing and coarse grid correction steps, we obtain a two grid iteration method.

Since the coarse grid correction problems are of the same type as the original one, we can apply the described fine-grid coarse-grid scheme recursively. Thereby, we obtain a multigrid method. The resulting coarse grid problems are approximately solved by one or two iteration steps (V-cycle or W-cycle). An exact computation of the coarse grid correction is carried out only on the coarsest grid. Smoothing steps are typically performed before and after the (approximate) determination of the coarse grid corrections.

This general concept forms the starting point for the development of various multigrid methods for solving the eigenproblem (7). These algorithms can roughly divided into two classes. The algorithms of the first class are characterized by using a linear multigrid method for the solution of linear problems arising from an outer iteration, whereas the algorithms of the second class are characterized by a direct application of the multigrid concept to the solution of problem (7).

We start with a short description of some methods of the first class. The algorithm of Bank [2] is based on inverse iteration. The arising linear systems are solved with a standard linear multigrid method. Bank and Chan [3] trace the computation of a simple eigenvalue back to a parameter dependent problem in the scalar parameter λ and use a multigrid continuation method for its solution. Hackbusch [14] regards the eigenproblem (7) as a nonlinear problem in the unknowns U and T which is solved by Newton's method. Here, the linear multigrid method for the solution of the linear subproblems is adapted to the special structure of the Jacobian.

Often, the multigrid concept is also used for preconditioning. In the selfadjoint case, there is a well known optimization method for the computation of the lowest eigenvalues with corresponding eigenfunctions: the simultaneous Rayleigh quotient minimization, see, e. g., Döhler [9]. In Jung et al. [15], this method is combined with a standard linear multigrid method for preconditioning. In this context, the algorithms suggested by Bramble et al. [4] and Leinen et al. [16] can be viewed as special types of the simultaneous Rayleigh quotient iteration with preconditioning.

Now we turn to the algorithms of the second class. First we describe the direct multigrid method of Hackbusch [13]. For convenience, we represent this method in the case of a simple eigenvalue computation. The equation

$$(A - \lambda_1 B)u_1 = 0 \tag{8}$$

is interpreted as a parameter dependent linear problem. For its solution, the multigrid idea is directly used in the following manner. At the beginning of every multigrid cycle, an approximation of the eigenvalue λ_1 is determined by computing the generalized Rayleigh quotient

$$\tilde{\lambda}_1 = \frac{\tilde{v}_1^* A \tilde{u}_1}{\tilde{v}_1^* B \tilde{u}_1} \quad ,$$

where \tilde{u}_1 and \tilde{v}_1 are approximations of the right and the left eigenvector. Then, this parameter value is fixed for the complete multigrid cycle. The smoother is a classical iteration method for the solution of linear problems, e. g., the Jacobi method or the Gauß-Seidel method. The coarse grid correction problems take the form

$$(A_l - \tilde{\lambda}_{1,l} B_l)w_l = d_l, \quad l = 0, \dots, l_{\max} - 1 \quad , \tag{9}$$

where the matrices A_l and B_l are the system and mass matrix corresponding to the finite element space V_l . The value $\tilde{\lambda}_{1,l}$ is an approximation of the eigenvalue $\lambda_{1,l}$ with lowest real part of this matrix pencil. The defect d_l results

from the current residue corresponding to the next higher level. For the unique solvability of equations (9), even in the case $\tilde{\lambda}_{1,l} = \lambda_{1,l}$, we must carry out projections of d_l and w_l with respect to the corresponding (approximate) eigenvector $\tilde{u}_{1,l}$ according to

$$\begin{aligned} d_l &\mapsto d_l^\perp = d_l - (\tilde{v}_{1,l}^* d_l) B_l \tilde{u}_{1,l} \\ w_l &\mapsto w_l^\perp = w_l - (\tilde{v}_{1,l}^* B_l w_l) \tilde{u}_{1,l} \quad , \end{aligned}$$

where $\tilde{v}_{1,l}$ is an approximation of the corresponding left eigenvector with $\tilde{v}_{1,l}^* B_l \tilde{u}_{1,l} = 1$. In our special case, the system matrices A_l are complex symmetric, and the mass matrices B_l are real symmetric, e. g., the left eigenvectors are the complex conjugate right eigenvectors. Hence, we can replace $\tilde{v}_{1,l}^*$ by $\tilde{u}_{1,l}^T$. Since we need approximations of the eigenpairs $(\lambda_{1,l}, u_{1,l})$ in every multigrid cycle, the use of a nested iteration technique is necessary. In case of the computation of an invariant subspace, a simultaneous iteration method is carried out for the solution of q equations of the form (8), for details see [13]. A proof of optimal complexity of Hackbusch's method is given in [12]. Another method of the second class is the nonlinear multigrid method, which is described in the paper [8] and the thesis [10]. Here, the essential idea for a direct multigrid approach for solving (7) is the successive solution of projected Schur problems

$$(V^* A V) W = (V^* B V) W T, \quad W^* (V^* B V) W = I \quad , \quad (10)$$

where the matrix V is given by

$$V = (\tilde{u}_1 \quad \cdots \quad \tilde{u}_q \quad p_1 \quad \cdots \quad p_r) \quad .$$

The vectors \tilde{u}_j are approximate Schur vectors, whereas the vectors p_k denote search directions. The matrices W and T are determined by an (approximate) partial Schur decomposition such that the diagonal of T consists of the q eigenvalues with lowest real parts of the matrix pencil $(V^* A V, V^* B V)$. Then, the new Schur vector approximations $U = (u_1 \quad \cdots \quad u_q)$ are given by $U = V W$. This general principle constitutes the foundation for the construction of both the smoothing algorithm and the coarse grid correction procedure. In the smoothing process the vectors p_k are chosen similarly to a one step block Arnoldi algorithm. One possible choice is, for instance,

$$(p_1 \quad \cdots \quad p_q) = P = A \tilde{U} - B \tilde{U} \tilde{T} \quad ,$$

where \tilde{T} is the upper triangular matrix corresponding to the current Schur vector approximations $(\tilde{u}_1 \quad \cdots \quad \tilde{u}_q) = \tilde{U}$. A more sophisticated choice is

described in [8, 10]. In the coarse grid correction procedure, the vectors p_k are the columns of the prolongation matrix P which describes the transition between the current coarse grid and the finest grid. If we realize the described idea in a multigrid recursion, the coarse grid problems are of the form

$$A_l W_l = B_l W_l T_l, \quad W_l^* B_l W_l = I \quad , \quad (11)$$

where the matrices A_l and B_l are the augmented system and mass matrices, respectively, according to (10). In contrast to the coarse grid problems (9) of Hackbusch's method, the matrices T_l in (11) (and hence the eigenvalue approximations $\lambda_{j,l}$) are also unknowns, which are automatically determined in the iteration process. Further, projections with respect to former determined eigenproblem solutions are not necessary.

In the case of a selfadjoint eigenproblem and computation of a simple eigenvalue, the just described method coincides with the Rayleigh quotient multigrid minimization of Mandel and McCormick [17, 19]. An important feature of this method is its monotonicity. This means, that the sequence of Rayleigh quotients formed in every step and at every stage of the algorithm decreases monotonically. Since the Rayleigh quotient is bounded from below, the sequence is always convergent. This property is the reason for the numerical robustness of the method. First optimal complexity results for the selfadjoint case are given by McCormick [20] and Cai et al. [5]. A simple, but illustrative numerical comparison between the Rayleigh quotient multigrid minimization and Hackbusch's method may be found in [7]. It turns out, that the Rayleigh quotient method is more robust, especially in the context of adaptivity. A different proof of optimality has been suggested by Chan and Sharapov [6] in connection with domain decomposition methods for the selfadjoint case. The theoretical investigation of the above nonlinear multigrid method for the computation of an invariant subspace, in particular for nonselfadjoint eigenproblems, and a proof of optimal complexity in this case are topics for future research.

4 Numerical Example

Now we return to the simple waveguide structure as shown in Figure 1. More complicated integrated optical components, even with amplified propagation (nonselfadjoint eigenproblem), may be found in [8, 10]. Here, we are only interested in the lowest eigenvalue with corresponding eigenfunction (fundamental mode of the structure).

The waveguide consists of a III-V-semiconductor material system (GaInAsP, InP). A cross section of the structure and the starting triangulation consisting

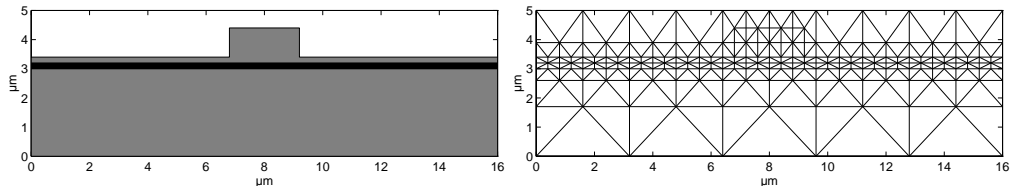


Figure 2: Cross section of the waveguide and starting triangulation.

of 206 nodes and 379 triangles are drawn in Figure 2. A simple manipulation shows that the function f in (4) can be represented as $f(x, y) = k_0^2 n^2(x, y)$, where k_0 is the wave number in vacuum, and the function $n(x, y)$ is given by the refractive indexes of the materials. Our computation is based on a wavelength of $1.55 \mu m$ (i. e. $k_0 = \frac{2\pi}{1.55} \approx 4.0537$) and the refractive indexes

$$n(x, y) = \begin{cases} 1.00, & \text{Air: white} \\ 3.17, & \text{InP: grey} \\ 3.38, & \text{GaInAsP: black} \end{cases}$$

taken from [1]. For the solution of this problem, we apply the nonlinear multigrid method as sketched in the preceding section and described in detail in [8, 10]. The adaptive meshes are constructed by a nested iteration technique in connection with a triangle based error indicator. The final tri-

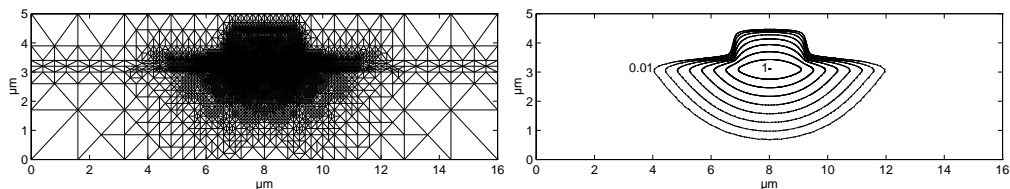


Figure 3: Final triangulation and logarithmic contour plot of the fundamental mode.

angulation with 12396 nodes and 24728 triangles reached after 7 refinements and a logarithmic contour plot of the computed eigenfunction u_1 are given in Figure 3. The corresponding eigenvalue is $\lambda_1 \approx -168.1927$, and the propagation number in z -direction is given by $k_1 = \sqrt{-\lambda_1} \approx 12.9689$. The discrete systems corresponding to each grid are solved with an accuracy of 10^{-5} in the residue. The whole computation with a MATLAB program takes 3 minutes on a Sun Ultra 1 workstation. The history of the full multigrid run is given in Table 1, whereas the effort in flops per grid is drawn in Figure 4.

Grid	1	2	3	4	5	6	7
Inner points	272	487	885	1743	3388	6437	12334
MG Iterations	6	6	7	7	7	6	7

Table 1: Number N of inner points and number of multigrid iterations per grid.

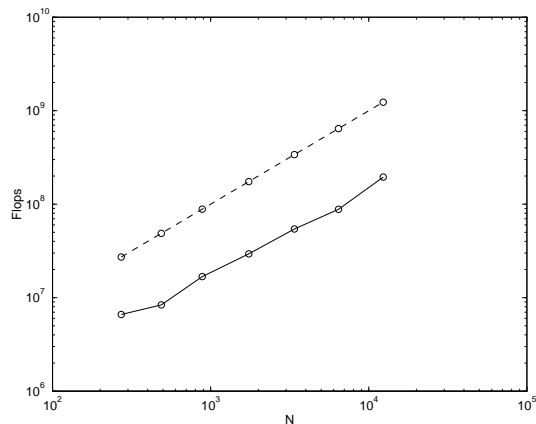


Figure 4: Log-log scale plot of flops versus N (compared with $10^5 N$: dashed line).

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