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A Multigrid Method for the Complex Helmholtz Eigenvalue Problem

Tilmann Friese[1], Peter Deuflhard[2], Frank Schmidt[3]

Introduction

The paper deals with the solution of the eigenvalue problem of the complex Helmholtz equation. We present an adaptive multigrid method for solving the nonselfadjoint algebraic eigenproblem arising from discretization with finite elements. A technological relevant numerical example, the simulation of an integrated optical component containing Multi Quantum Well layers, is included.

The task is to find a few eigenvalues λ and corresponding eigenfunctions u of the Helmholtz equation with Dirichlet boundary condition

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

where the region Ω is an open, bounded, and connected subset of $\mathbf{R}^2$, and the function f is bounded and in general complex valued. As usual, we transform this problem in its weak formulation: determine $u \in H_0^1(\Omega) \setminus \{0\}$ and $\lambda \in \mathbf{C}$, such that the relation

$$a(v,u) = \lambda\,(v,u) \quad \forall v \in H_0^1(\Omega) \tag{1}$$

1 Konrad-Zuse-Zentrum für Informationstechnik Berlin, Takustr. 7, D-14195 Berlin, Germany, E-mail: friese@zib.de. Research supported by the BMBF under grant 03-DE7ZIB-5.

2 Address same as above, E-mail: deuflhard@zib.de.

3 Address same as above, E-mail: frank.schmidt@zib.de.

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with the sesquilinear form $a(v,u) = (\nabla v, \nabla u) - (v, fu)$ is fulfilled. The inner product $(\cdot,\cdot)$ is herein given by the L^2 scalar product. In the special case of a pure real valued function f the eigenvalue problem (1) is selfadjoint. In the general case of a complex valued function f we have to solve a nonselfadjoint eigenproblem. Finally, in many cases the eigenvalues with lowest real parts and the corresponding eigenfunctions are of interest.

By using the Rayleigh quotient

$$R(u) = \frac{a(u,u)}{(u,u)}$$

we can conclude from a simple computation [Sch95] that the eigenvalues λ lie in a half stripe Σ of the complex plane as shown in Figure 1. Furthermore, from a general

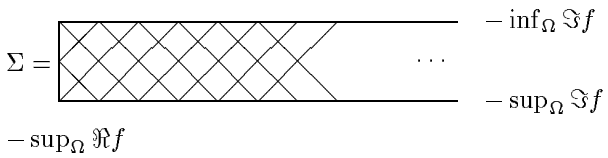

Figure 1 Position of the eigenvalues in the complex plane.

completeness result of KATSNELSON [Kat67] we obtain the following

Theorem 1. *Let the region Ω and the function f be given as above. Then the spectrum of the associated Helmholtz operator is discrete, and there exists a basis $\{u_j\}_{j=1}^{\infty}$ of $L^2(\Omega)$, such that the relation*

$$a(v,u_j) = \lambda_j\,(v,u_j) + \sum_{k=1}^{j-1} \tau_{kj}\,(v,u_k) \quad \forall v \in H_0^1(\Omega) \tag{2}$$

holds. The eigenvalues fulfill the inequalities $\Re\lambda_1 \le \Re\lambda_2 \le \ldots \to \infty$.

Remark 1. In the special selfadjoint case the COURANT minimax principle [CH53] shows that this basis is even orthonormal. In addition, the values τ_{kj} are zero, i. e., the basis consists only of eigenfunctions.

The statements of Theorem 1 enable us to carry out a perturbation analysis as for matrix eigenvalue problems, see, e. g., [GV89]. It turns out that the sensitivity of the eigensolutions with respect to perturbations in f depends on the spectral gap, i. e., on the separation of the eigenvalues from the remaining part of the spectrum. We can conclude that we should determine the interesting eigensolutions in terms of invariant subspaces.

The discretization of (2) with finite elements leads to the generalized matrix eigenvalue problem

$$AU = BUT \tag{3}$$

with the sparse system matrix A, the sparse, selfadjoint, and positive definite mass matrix B, and the unknown matrices U and T. The column vectors of the matrix U represents a basis of the interesting discrete invariant subspace. From the partial Schur decomposition of matrices [GV89] we see that the matrix U may be chosen orthonormal, i. e., $U^*BU = I$, and that the matrix T is upper triangular with the discrete eigenvalues in the diagonal. It can be shown [Fri98] that the discrete eigenvalues lie also in the half stripe Σ of the complex plane. Furthermore, in the selfadjoint case the upper triangular matrix T reduces to a diagonal one. Hence the discrete problem (3) reflects all properties of the continuous problem.

A Multigrid Method for the Helmholtz Eigenproblem

In this section we present a multigrid algorithm for the efficient solution of the discrete eigenproblem (3). We restrict ourselves to conforming methods, i. e., we assume a nested sequence of finite element spaces

$$S_0 \subset S_1 \subset \ldots \subset S_{l_{\max}} \subset H_0^1(\Omega) \quad .$$

We begin with the description of the multigrid principle for the special selfadjoint case. The starting point of our considerations is the following minimal property of the invariant subspace corresponding to the q lowest eigenvalues: the matrix U is given as the minimal point

$$R(U) = \min_V R(V)$$

of the generalized Rayleigh quotient $R(V) = \operatorname{trace}\big((V^*BV)^{-1}(V^*AV)\big)$, where the matrix V has q columns and full rank. This characterization leads to the following general algorithmic idea: given an approximation $\widetilde{U}$ of U and search directions $\widetilde{P}$, determine a new approximation $\widehat{U}$ by minimization of the generalized Rayleigh quotient over the subspace spanned by the column vectors of the matrices $\widetilde{U}$ and $\widetilde{P}$, i. e., by

$$R(\widehat{U}) = \min_{\binom{\Phi}{\Psi}} R(\widetilde{U}\Phi + \widetilde{P}\Psi) \quad , \tag{4}$$

where the matrix $\binom{\Phi}{\Psi}$ has q columns and full rank. If we iterate this procedure we obtain an algorithm which traces the solution of the original large scale problem back to the successive solution of low dimensional problems of the same type. This general method produces a sequence of invariant subspace approximations with decreasing functional values, i. e., it is a monotone method.

From this general principle we can derive a multigrid algorithm for the selfadjoint case. The resulting method is a generalization of the multigrid minimization of Mandel, McCormick [MM89] to invariant subspace computations. In the smoothing step we apply a classical Rayleigh quotient minimization method such as, e. g., a simultaneous gradient [LM80] or conjugate gradient method [Döh82]. This means, the matrix $\widetilde{P}$ of search directions is formed by the gradient or by a generalized conjugate gradient of the Rayleigh quotient. The numerical experience shows that these algorithms have a smoothing property. Furthermore, in the coarse grid correction step the matrix $\widetilde{P}$ is given by the usual prolongation matrix which describes the

transition between the coarse and the fine grid. Hence both parts of the multigrid algorithm are based on the above described minimization principle which implies the monotonicity of the method. This property ensures a high numerical robustness of the algorithm.

Remark 2. Optimal complexity results for a variant of the described method with a different smoothing procedure were given by McCormick [McC94] and Cai, Mandel, McCormick [CMM97]. A different proof of optimality has been suggested by Chan, Sharapov [CS96] in connection with domain decomposition techniques. A numerical comparison between the multigrid minimization and the multigrid method of Hackbusch [Hac85] in the context of adaptive generated meshes may be found in [DFS+96]. It turns out that, on one hand, the above described method is more robust, and, on the other hand, the two methods have asymptotically the same convergence rates.

For the generalization of the above method to the nonselfadjoint case we use the fact that the solution of the minimization problem (4) is equivalent to the solution of an eigenvalue problem

$$\widetilde{A}\Theta = \widetilde{B}\Theta\widehat{\Lambda}$$

with the projected matrices

$$\widetilde{A} = \begin{pmatrix} \widetilde{U} & \widetilde{P} \end{pmatrix}^* A \begin{pmatrix} \widetilde{U} & \widetilde{P} \end{pmatrix} \quad \text{and} \quad \widetilde{B} = \begin{pmatrix} \widetilde{U} & \widetilde{P} \end{pmatrix}^* B \begin{pmatrix} \widetilde{U} & \widetilde{P} \end{pmatrix} \quad .$$

The essential idea for the extension of the multigrid minimization to nonselfadjoint problems is to replace these projected eigenvalue problems in each smoothing and coarse grid correction step by projected Schur problems

$$\widetilde{A}\Theta = \widetilde{B}\Theta\widehat{T} \quad .$$

By this modification, we obtain the following smoothing algorithm which resembles a Block Arnoldi method [Saa92].

Algorithm 1.

- Initialization:
  - given a $(N \times q)$-matrix U with $U^*BU = I$, $U^*AU = T_U$
  - set $P = R = -(AU - BUT_U)$
- Iteration:
  - set $V = \begin{pmatrix} U & P \end{pmatrix}$
  - solve
$$\begin{aligned} (V^*AV)\Theta &= (V^*BV)\Theta T \\ \Theta^*(V^*BV)\Theta &= I \end{aligned}$$
    with $\Re(\lambda_1) \le \ldots \le \Re(\lambda_q) < \Re(\lambda_{q+1}) \le \ldots \le \Re(\lambda_{2q})$
  - set $\begin{pmatrix} U & P \end{pmatrix} = V\Theta$
  - compute $R = -(AU - BUT_U)$

* determine X from

$$XT_U - T_P X = P^*(AR - BRT_U)$$

  with $T_P = P^*AP$
* set $P = R + PX$

A detailed description of this procedure is given in [DFS97, Fri98]. Again, the numerical experience shows that this method has a smoothing property. Furthermore, as above, the search directions in the coarse grid correction step are given by the usual prolongation matrix. Since, in particular, the arising coarse grid problems are of the same type as the original problem (3), a recursive application of a multigrid procedure as given in Algorithm 2 is possible.

Algorithm 2.

$[U_l, T_l] = \mathrm{MGM}(A_l, B_l, U_l, T_l, l)$

1. presmoothing using Algorithm 1: $U_l \to \widetilde{U}_l$, $T_l \to \widetilde{T}_l$
2. coarse grid correction: $\widetilde{U}_l \to \widehat{U}_l$, $\widetilde{T}_l \to \widehat{T}_l$
   - compute $A_{l-1} = V_l^* A_l V_l$ and $B_{l-1} = V_l^* B_l V_l$, where in case
     * $l = l_{\max}$: $V_l = \begin{pmatrix} \widetilde{U}_l & P_l \end{pmatrix}$
     * $l < l_{\max}$: $V_l = \begin{pmatrix} \widetilde{U}_l & 0 \\ & P_l \end{pmatrix}$
   - if
     * $l > 1$: $[U_{l-1}, T_{l-1}] = \mathrm{MGM}(A_{l-1}, B_{l-1}, \begin{pmatrix} I \\ 0 \end{pmatrix}, \widetilde{T}_l, l-1)$
     * $l = 1$: solve
$$\begin{aligned} A_0 U_0 &= B_0 U_0 T_0 \\ U_0^* B_0 U_0 &= I \end{aligned}$$
   - set $\widehat{U}_l = V_l U_{l-1}$, $\widehat{T}_l = T_{l-1}$
3. postsmoothing using Algorithm 1: $\widehat{U}_l \to U_l$, $\widehat{T}_l \to T_l$

In Algorithm 2, the matrices A_l and B_l are the (augmented) system and mass matrix corresponding to the finite element space S_l. The matrix U_l with q columns and the upper triangular matrix T_l are the matrices of unknowns. The matrix P_l is the prolongation matrix for the interpolation between the spaces S_l and S_{l-1}.

Remark 3. Note, that this multigrid method for the nonselfadjoint case is not based on a minimization principle. An elaborate theoretical investigation of the method, especially a proof of optimality, is an open topic for future research. However, numerical experiments as presented in the following section suggest the optimal complexity of the algorithm.

Numerical Example

For the illustration of the performance of the above described multigrid algorithm we have computed the guided modes of an integrated optical component which is invariant in z-direction. The cross section of the interesting structure is drawn in Figure 2. The

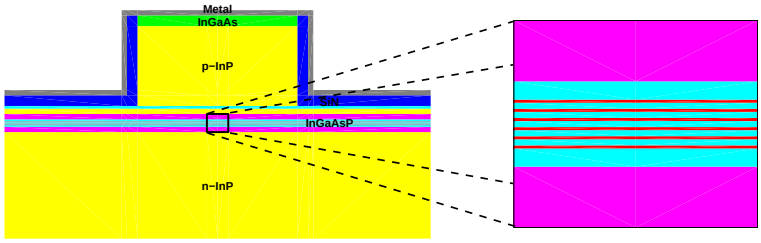

Figure 2 Cross section of an integrated optical structure with zoom.

function f can be represented as $f(x,y) = k_0^2 n^2(x,y)$, where k_0 is the vacuum wave number of light, and the function $n(x,y)$ is given by the refractive indexes of the materials. The refractive index is complex valued and parameter dependent in the Multi Quantum Well (MQW) layers (the narrow stripes in the zoom of Figure 2), complex valued in the metal layer, and real valued otherwise. The exact parameters of the structure are technologically relevant and therefore not documented here.

For the construction of the hierarchy of meshes we used a nested iteration technique in connection with a triangle based error indicator. At first, for each triangle t_j a relative L^2 error ε_j with respect to the whole invariant subspace was determined by computation of a correction in the edge midpoints of the current triangulation with a scheme analogously to the Jacobi method for linear systems. Then, the triangles t_k with

$$\varepsilon_k > \frac{1}{2} \max \varepsilon_j$$

were refined uniformly, and neighbouring triangles were divided by a bisection method to remove hanging nodes.

In a first experiment, we were interested in the two eigenvalues with lowest real parts and their corresponding Schur functions. A difficulty of this problem was to find a proper starting triangulation. Since we must resolve the very thin MQW layers with normally sized triangles, the coarsest mesh (shown in Figure 3) consists already of 2515 nodes and 4956 triangles. The final triangulation with 15246 nodes and 30396 triangles reached after 6 refinements is also given in Figure 3. The numerical experiments have been performed with a tolerance $\mathrm{tol} = 10^{-3}$ for all multigrid levels. The whole computation with a MATLAB program took 16 minutes on a SUN ULTRA 1 workstation. The coarsest grid problems were solved with a Block Arnoldi procedure [Saa92]. Logarithmic contour plots for the resulting Schur functions on the final mesh are represented in Figure 4. The convergence history of the full multigrid run is given

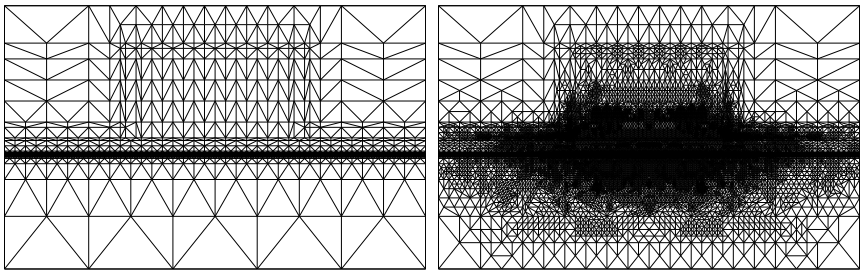

Figure 3 Starting and final triangulation.

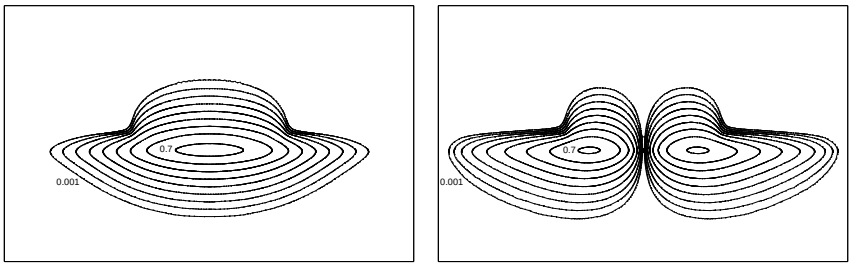

Figure 4 Logarithmic contour plots of $|u_1|^2$ and $|u_2|^2$.

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

Grid	1	2	3	4	5	6
Inner points	2564	2888	3987	5536	9422	15152
MG Iterations	3	3	4	4	4	4

in Table 1.

In a second experiment, we carried out a parameter study to demonstrate the dependence of the eigenvalues on the imaginary part of the refractive index in the MQW layers. We computed the invariant subspace corresponding to the four eigenvalues with lowest real parts for the parameter values $\alpha = 0, 0.25, 0.5, 0.75, 1$. The computed eigenvalue trajectories are shown in Figure 5. The two eigenvalues from the previous computation are marked with arrows. This type of diagram is of technological interest.

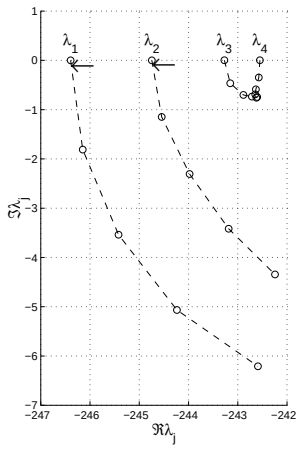

Figure 5 Dependence of the eigenvalues on the imaginary part of the refractive index in the Multi Quantum Well layers.

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REFERENCES

[CH53] Courant R. and Hilbert D. (1953) *Methods of Mathematical Physics*, volume 1. Wiley Interscience New York.

[CMM97] Cai Z., Mandel J., and McCormick S. F. (1997) Multigrid methods for nearly singular linear equations and eigenvalue problems. *SIAM J. Numer. Anal.* 34: 178–200.

[CS96] Chan T. F. and Sharapov I. (1996) Subspace correction multilevel methods for elliptic eigenvalue problems. CAM Report 96-34, University of California Los Angeles.

[DFS+96] Deuflhard P., Friese T., Schmidt F., März R., and Nolting H.-P. (1996) Effiziente Eigenmodenberechnung für den Entwurf integriert-optischer Chips. In Hoffmann K.-H., Jäger W., Lohmann T., and Schunck H. (eds) *Mathematik-*

Schlüsseltechnologie für die Zukunft, pages 267–280. Springer-Verlag Berlin Heidelberg New York.

[DFS97] Deuflhard P., Friese T., and Schmidt F. (1997) A nonlinear multigrid eigenproblem solver for the complex Helmholtz equation. Preprint SC 97-55, Konrad-Zuse-Zentrum für Informationstechnik Berlin.

[Döh82] Döhler B. (1982) Ein neues Gradientenverfahren zur simultanen Berechnung der kleinsten oder größten Eigenwerte des allgemeinen Eigenwertproblems. *Numer. Math.* 40: 79–91.

[Fri98] Friese T. (1998) *Eine Mehrgitter-Methode zur Lösung des Eigenwertproblems der komplexen Helmholtzgleichung*. PhD thesis, Freie Universität Berlin.

[GV89] Golub G. H. and Van Loan C. F. (1989) *Matrix Computations*. The Johns Hopkins University Press Baltimore London, second edition.

[Hac85] Hackbusch W. (1985) *Multi-Grid Methods and Applications*. Springer-Verlag Berlin Heidelberg New York.

[Kat67] Katsnelson V. E. (1967) Conditions under which systems of eigenvectors of some classes of operators form a basis. *Funct. Anal. Appl.* 1: 122–132.

[LM80] Longsine D. E. and McCormick S. F. (1980) Simultaneous Rayleigh-quotient minimization methods for $Ax = \lambda Bx$. *Lin. Alg. Appl.* 34: 195–234.

[McC94] McCormick S. F. (1994) Multilevel adaptive methods for elliptic eigenproblems: A two-level convergence theory. *SIAM J. Numer. Anal.* 31: 1731–1745.

[MM89] Mandel J. and McCormick S. F. (1989) A multilevel variational method for $Au = \lambda Bu$ on composite grids. *J. Comp. Phys.* 80: 442–452.

[Saa92] Saad Y. (1992) *Numerical Methods for Large Eigenvalue Problems*. Manchester University Press.

[Sch95] Schmidt F. (1995) Simultaneous computation of the lowest eigenvalues and eigenvectors of the Helmholtz equation. Technical Report TR 95-13, Konrad-Zuse-Zentrum für Informationstechnik Berlin.