EFFICIENT NUMERICAL SOLUTION OF LARGE SPARSE EIGENVALUE PROBLEMS IN MICROELECTRONIC LASER DESIGN

Thomas Kerkhoven and Albert T. Galick,
Department of Computer Science,
University of Illinois at Urbana–Champaign, Urbana, IL 61801,

Umberto Ravaioli,
Beckman Institute and Coordinated Science Laboratory,
University of Illinois at Urbana–Champaign, Urbana, IL 61801.

Abstract

The propagation of an electromagnetic wave through a variable complex dielectric wave-guiding medium is modeled by the two transverse components of the magnetic field on a two dimensional domain, perpendicular to the propagation direction. The large sparse complex non-hermitian eigenvalue problem for the spurious–mode–free discretization is solved very efficiently by an iterative Chebyshev–Arnoldi algorithm. The key to this efficiency is an analysis of the eigenvalue problem in which the location of the nonbound spectrum and the rapidly attenuating modes is determined a priori. The eigenvalues corresponding to bound modes are selectively enhanced by suitable adaptation of the Chebyshev acceleration. The nonbound modes and the rapidly attenuating bound modes are removed in an outer iteration. This dual strategy of pre-conditioning and selection rapidly isolates those few modes (typically less than 20) which are relevant from an engineering point of view.

1 Introduction

We present a computational approach to the solution of two–dimensional eigenvalue problems in semiconductor laser simulation based on an efficient implementation of the iterative Chebyshev–Arnoldi algorithm. Our approach greatly reduces memory requirements because it allows the matrix of the discretized problem to be stored in sparse form. The computational complexity is reduced significantly by computing only those eigenvalues and eigenvectors which correspond to propagating modes properly confined to the active region of the laser. This allows us to employ extensive nonuniform meshes with many grid points on which the discretization error can be controlled.

Following the approach in [1], we discretize the electromagnetic wave equation

$$-\frac{1}{\epsilon(x,y)}\nabla^2\vec{H} + \nabla\frac{1}{\epsilon(x,y)} \times (\nabla \times \vec{H}) = \omega^2\mu\vec{H}, \tag{1}$$

where the relative permittivity $\epsilon(x,y)$ is complex. Assuming an axial dependence of $e^{i\beta z}$ yields a complex nonhermitian generalized eigenvalue problem, $Ku = -\beta^2 Mu$. Here u is formed by concatenating H_x and H_y in the standard grid ordering. Thus K has two diagonal blocks of five bands each for H_x and H_y, and two off–diagonal blocks of three bands each for the coupling terms. On the right hand side M is a positive diagonal matrix. This generalized eigenvalue problem is recast as a standard eigenvalue problem, $Av = -\beta^2 v$, where $A = M^{-1/2}KM^{-1/2}$ and $v = M^{1/2}u$.

2 Solution of the Eigenvalue Problem

In our computations we use a uniform grid in the core region. The mesh spacing grows exponentially as the lines extend far out into the cladding. Such grids both resolve rapid oscillations of higher modes in the core region and extend sufficiently far to allow the modes to decay exponentially into the cladding. With two complex field components at each grid point, such grids give rise to very large scale eigenvalue problems. However, only a few eigenvalues correspond to confined, propagating modes. To characterize propagation in terms of the eigenvalue, we write $-\beta^2 = \xi + i\zeta = -(\eta + i/L)^2$, so that the axial dependence $e^{i\beta z}$ has real part $e^{-z/L}$, indicating a characteristic propagation length L. As will be shown elsewhere, the propagating modes then satisfy

$$\frac{1}{L^2} = \frac{\xi + \sqrt{\xi^2 + \zeta^2}}{2} < \frac{1}{L_0^2}, \tag{2}$$

where L_0 is the minimum acceptable propagation length.

To characterize the confined modes, we focus our attention on the cladding, where we may use the scalar Helmholtz equation for H_z

$$\frac{1}{\rho}\partial_\rho(\rho\partial_\rho H_z) + \frac{1}{\rho^2}\partial_{\theta\theta}H_z + (\omega^2\mu\epsilon - \beta^2)H_z = 0. \tag{3}$$

The switch to the scalar equation in polar coordinates is to clarify the discussion—this is a quick study rather than a rigorous proof. In this spirit, we assume a solution in the cladding with radial dependence $e^{-(1/\tau + i\kappa)\rho}$, i.e., a characteristic transverse confinement length τ. Then Eq. (3) becomes $(1/\tau + i\kappa)^2 H_z - (1/\tau + i\kappa)H_z/\rho + \partial_{\theta\theta}H_z/\rho^2 + (\omega^2\mu\epsilon - \beta^2)H_z = 0$. As will be shown elsewhere, the confined modes then satisfy

$$\frac{1}{\tau^2} = \frac{-\omega^2\mu\epsilon_{\text{clad}} - \xi + \sqrt{(\omega^2\mu\epsilon_{\text{clad}} + \xi)^2 + \zeta^2}}{2} > \frac{1}{\tau_0^2}, \tag{4}$$

where τ_0 is the maximum acceptable transverse confinement length and ϵ_{clad} is the maximum permittivity attained on a significant section of cladding.

We use an iterative Chebyshev preconditioned Krylov subspace method to converge specifically to these confined modes. We precondition with the Chebyshev polynomial adapted to the reference ellipse through λ_r,

$$p_n(\lambda) = T_n\left(\frac{\lambda - d}{c}\right) \Big/ T_n\left(\frac{\lambda_r - d}{c}\right).$$

We use a reference ellipse tangent to the confinement cutoff parabola with $\lambda_r = -\omega^2\mu\epsilon_{\text{clad}} - 1/\tau_0^2$, left focus $d - c = -\omega^2\mu\epsilon_{\text{clad}}$, and right focus $d + c$ an upper bound for the spectrum, as determined by Gerschgorin disks.

As n increases, $|p_n(\lambda)|$ approaches $[\kappa(\lambda)]^n$, where

$$\kappa(\lambda) = \frac{a(\lambda) + (a(\lambda)^2 - c^2)^{1/2}}{a(\lambda_r) + (a(\lambda_r)^2 - c^2)^{1/2}}$$

and $a(\lambda)$ is the major semiaxis of the ellipse through λ with center d and real foci $d - c$, $d + c$ [2, 3]. Thus, the strength of the preconditioning of λ depends on the distance between the confocal ellipses through λ and λ_r. The efficient computation of matrix–vector products of the form $v_n = [p_n(A)]v_0$ is described in [1].

The Chebyshev–Arnoldi algorithm generates an orthonormal basis V_m for the Krylov subspace $K_m[p_n(A), v_0] = \text{span}\{v_0, [p_n(A)]v_0, [p_n(A)]^2 v_0, \ldots, [p_n(A)]^{m-1}v_0\}$. The Chebyshev polynomial

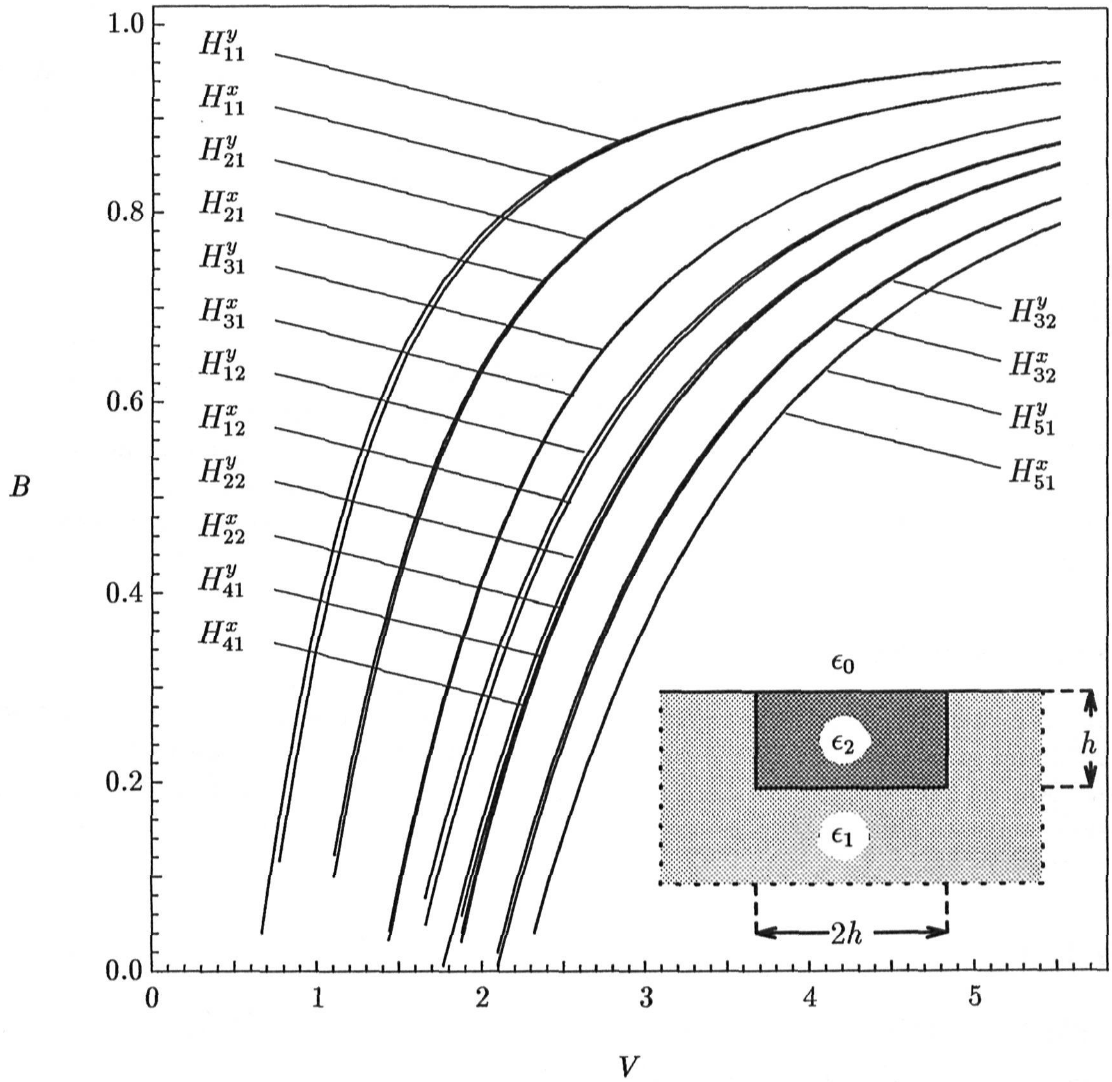

Figure 1: Channel waveguide. Normalized propagation constant $B = \dfrac{(\beta/k_0)^2 - \epsilon_1}{\epsilon_2 - \epsilon_1}$ vs. normalized frequency $V = (2h/\lambda)(\epsilon_2 - \epsilon_1)^{1/2}$, with k_0 the free–space wavenumber. The computational domain is 60μm $\times$ 32μm, with $h = 3\mu$m, $\epsilon_1 = 2.13\epsilon_0$ and $\epsilon_2 = 2.25\epsilon_0$. The discretization is on a 69×38 nonuniform rectangular grid.

preconditioning greatly magnifies the separation of the eigenvalues satisfying Ineq. (4) relative to the rest of the spectrum, while leaving the eigenvectors unchanged. Convergence towards the desired eigenvectors is thus accelerated [4]. After finding the orthonormal basis V_m, we take a Rayleigh quotient $C_m = V_m^* A V_m$ of the operator A over the Krylov subspace. The spectral decomposition $C_m = Y_m \Lambda_m Y_m^{-1}$ is found using standard EISPACK routines. The approximate eigenvalues and eigenvectors of A are then Λ_m and $V_m Y_m$. The best confined of these (i.e, those with smallest τ) satisfying both the confinement and propagation conditions Ineq. (4) and (2) are combined into a new starting vector v_0, and the whole process is repeated with stronger preconditioning, i.e., polynomials of higher degree n, until the residuals are within a prescribed tolerance. We have found this outer iteration to be effective in removing unwanted modes. For typical problems, as in Fig. 1 on a 69×38 mesh, convergence to the few confined modes takes a few dozen outer iterations for a total of about 25 CPU minutes on a Sparc 2. In the near future we plan to incorporate this solver in the laser simulation package MINILASE [5].

3 Conclusion

Realistic modeling of microelectronic lasers requires the solution of complex eigenvalue problems that are very large and sparse. The approach for the real nonsymmetric eigenvalue problem, presented in [1], easily generalizes to the complex nonhermitian eigenvalue problem in laser simulation. In our approach, only the eigenvectors for propagating, confined, modes are computed. The Chebyshev–preconditioned Arnoldi projection method has been demonstrated to be very suitable for this application.

4 Acknowledgements

The authors gratefully acknowledge support by the Office of Naval Research grant SDI–IST N00014-90–J–1270 and grants NSF ECS 912–0641 and NSF ECD 89–43166. We are highly indebted to Professor Ahmed Sameh who gave significant support over the course of this project in many useful discussions and who allowed us to use the facilities of the Center for Supercomputing Research and Development.

References

[1] A. Galick, T. Kerkhoven, and U. Ravaioli, *IEEE Trans. MTT* **40**, 699 (1992).

[2] Y. Saad, *Math. Comp.* **42**, 567 (1984).

[3] D. Ho, F. Chatelin, and M. Bennani, *Math. Model. Numer. Anal.* **24**, 53 (1990).

[4] Y. Saad, In *Matrix Pencils, Proceedings*, 121, (Springer-Verlag, 1982).

[5] G. H. Song, K. Hess, T. Kerkhoven, and U. Ravaioli, *Europ. Trans. on Telecom.* **1**, 375 (1990).