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A JACOBI–DAVIDSON ALGORITHM FOR LARGE EIGENVALUE PROBLEMS FROM OPTO-ELECTRONICS

* Peter Arbenz[1], Christof Vömel[2], and Ratko G. Vepřek[3]

[1] ETH Zurich
Institute of Computational Science
CH-8092 Zurich
arbenz@inf.ethz.ch

[2] ETH Zurich
Institute of Computational Science
voemel@inf.ethz.ch

[3] ETH Zurich
Integrated Systems Laboratory
veprek@iis.ee.ethz.ch

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ABSTRACT

The construction of prototypes of nowadays opto-electronic components during their development is very expensive. Therefore, they are developed and simulated on the computer. This procedure admits to determine and optimize their characteristics, in particular their optical characteristics, in advance. The progressive miniaturization of opto-electronic components leads to numerous quantum-mechanical effects, that cannot be treated by the usual classical models. Quantum-mechanical methods have to be employed. The states of the charge carriers and the dispersion relations are determined by coupled Schrödinger equations. Their discretization by means of the finite element method leads to large sparse generalized complex Hermitian matrix eigenvalue problems. If multiple bands of the electronic band structure are simulated by the $\mathbf{k}\cdot\mathbf{p}$ method the matrix becomes indefinite.

Because of their size the solution of these eigenvalue problems requires sophisticated eigensolvers. We present a variant of the Jacobi–Davidson (JD) algorithm that is based on a real symmetric formulation of the complex Hermitian eigenvalue problem. The correction equations that have to be solved in each step of JD are solved by a conjugate gradient-type algorithm preconditioned by a V-cycle of smoothed aggregation multigrid. In the indefinite case the spectrum is folded to arrive at positive definite problems.

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