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Multilevel preconditioned iterative eigensolvers for Maxwell eigenvalue problems

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Abstract

We investigate eigensolvers for computing a few of the smallest eigenvalues of a generalized eigenvalue problem resulting from the finite element discretization of the time independent Maxwell equation. Various multilevel preconditioners are employed to improve the convergence and memory consumption of the Jacobi–Davidson algorithm and of the locally optimal block preconditioned conjugate gradient (LOBPCG) method. We present numerical results of very large eigenvalue problems originating from the design of resonant cavities of particle accelerators.

Keywords: Maxwell equation; Generalized eigenvalue problem; Jacobi–Davidson; LOBPCG; Smoothed aggregation AMG preconditioner

1. Introduction

Many applications in electromagnetics require the computation of some of the eigenpairs of the curl–curl operator,

$$\mathbf{curl}\,\mu_r^{-1}\,\mathbf{curl}\,\mathbf{e}(\mathbf{x}) - k_0^2\varepsilon_r\mathbf{e}(\mathbf{x}) = \mathbf{0}, \qquad \operatorname{div}\mathbf{e}(\mathbf{x}) = 0, \quad \mathbf{x}\in\Omega, \tag{1.1}$$

in a bounded simply-connected, three-dimensional domain Ω with homogeneous boundary conditions $\mathbf{e}\times\mathbf{n} = \mathbf{0}$ posed on the connected boundary $\partial\Omega$. Here, ε_r and μ_r are the relative permittivity and permeability, respectively. Eq. (1.1) are obtained from the Maxwell equations after separation of the time

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and space variables and after elimination of the magnetic field intensity. While ε_r and μ_r are complex numbers in problems from waveguide or laser design, in simulation of accelerator cavities the materials can be assumed to be loss-free, thus admitting real ε_r and μ_r, whence all eigenvalues are real. In fact, we will assume $\varepsilon_r = \mu_r = 1$. Thus, the discretization of (1.1) by finite elements leads to a real symmetric generalized matrix eigenvalue problem

$$A\mathbf{x} = \lambda M\mathbf{x}, \qquad C^{\mathrm{T}}\mathbf{x} = \mathbf{0}, \tag{1.2}$$

where A is positive semidefinite and M is positive definite. In this paper we consider eigensolvers for computing a few, i.e., five to ten of the smallest eigenvalues and corresponding eigenvectors of (1.2) as efficiently as possible with regard to execution time and consumption of memory space. In earlier studies [1,2] we found the Jacobi–Davidson algorithm [28] and the locally optimal block preconditioned conjugate gradient (LOBPCG) method [19] to be the most effective solvers for this task. We now have incorporated a sophisticated multilevel preconditioner that is the combination of a hierarchical basis [4] and a smoothed aggregation AMG preconditioner [30,26]. We review eigensolvers and preconditioners and tell how we employ them in Sections 3 to 4. In Section 5 we report on experiments that we conducted by means of problems originating in the design of the RF cavity of the 590 MeV ring cyclotron installed at the Paul Scherrer Institute (PSI) in Villigen, Switzerland. These experiments indicate that the implemented multilevel preconditioner is indeed optimal in that the number of iteration steps until convergence only slightly depends on the problem size.

2. The application: The cavity eigenvalue problem

The finite element discretization is based on the weak formulation of (1.1) as suggested in [18]:

$$\begin{aligned}
&\text{Find } (\lambda_h, \mathbf{e}_h, p_h) \in \mathbb{R} \times N_h \times L_h \text{ such that } \mathbf{e}_h \neq \mathbf{0} \text{ and} \\
&\text{(a) } (\mathbf{curl}\,\mathbf{e}_h, \mathbf{curl}\,\boldsymbol{\Psi}_h) + (\mathbf{grad}\,p_h, \boldsymbol{\Psi}_h) = \lambda_h(\mathbf{e}_h, \boldsymbol{\Psi}_h), \quad \forall \boldsymbol{\Psi}_h \in N_h, \\
&\text{(b) } (\mathbf{e}_h, \mathbf{grad}\,q_h) = 0, \qquad\qquad\qquad\qquad\quad \forall q_h \in L_h,
\end{aligned} \tag{2.1}$$

where $N_h \subset H_0(\mathbf{curl}; \Omega) = \{\mathbf{v} \in L^2(\Omega)^3 \mid \mathbf{curl}\,\mathbf{v} \in L^2(\Omega)^3, \mathbf{v} \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega\}$ and $L_h \subset H_0^1(\Omega)$. In order to avoid spurious modes we choose the subspaces N_h and L_h, respectively, to be the Nédélec (or edge) elements [14,27] and the Lagrange (or node-based) finite elements [6] both of matching degree, in our implementation of degree 2. Let $\{\boldsymbol{\Phi}_i\}_{i=1}^n$ be a basis of N_h and $\{\varphi_l\}_{l=1}^m$ be a basis of L_h. Then (2.1) defines the matrix eigenvalue problem

$$\begin{bmatrix} A & C \\ C^{\mathrm{T}} & O \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \lambda \begin{bmatrix} M & O \\ O & O \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}, \tag{2.2}$$

respectively, where A and M are n-by-n and C is n-by-m with elements

$$a_{i,j} = (\mathbf{curl}\,\boldsymbol{\Phi}_i, \mathbf{curl}\,\boldsymbol{\Phi}_j), \qquad m_{i,j} = (\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j), \qquad c_{i,l} = (\boldsymbol{\Phi}_i, \mathbf{grad}\,\varphi_l).$$

Eq. (2.2) can equivalently be written in the form (1.2). The reason for approximating the electric field $\mathbf{e}$ by Nédélec elements and the Lagrange multipliers by Lagrange finite elements is that [14, §III.5.3]

$$\mathbf{grad}\,L_h = \{\mathbf{v}_h \in N_h \mid \mathbf{curl}\,\mathbf{v}_h = \mathbf{0}\}. \tag{2.3}$$