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Preconditioning bandgap eigenvalue problems in three-dimensional photonic crystals simulations

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ABSTRACT

To explore band structures of three-dimensional photonic crystals numerically, we need to solve the eigenvalue problems derived from the governing Maxwell equations. The solutions of these eigenvalue problems cannot be computed effectively unless a suitable combination of eigenvalue solver and preconditioner is chosen. Taking eigenvalue problems due to Yee's scheme as examples, we propose using Krylov–Schur method and Jacobi–Davidson method to solve the resulting eigenvalue problems. For preconditioning, we derive several novel preconditioning schemes based on various preconditioners, including a preconditioner that can be solved by Fast Fourier Transform efficiently. We then conduct intensive numerical experiments for various combinations of eigenvalue solvers and preconditioning schemes. We find that the Krylov–Schur method associated with the Fast Fourier Transform based preconditioner is very efficient. It remarkably outperforms all other eigenvalue solvers with common preconditioners like Jacobi, Symmetric Successive Over Relaxation, and incomplete factorizations. This promising solver can benefit applications like photonic crystal structure optimization.

1. Introduction

Photonic crystals are periodic dielectric structures with a frequency region and specific band structures and they have been studied extensively from both theoretical and practical aspects. Numerical simulations that are based on the solutions of the time harmonic Maxwell's equations have also played an important role among the studies. Some spatial discretization methods include the finite difference methods [11,12,32,50], the finite volume methods [13,14,31], the finite element methods [7,9,10,16,27,34], the Whitney form [6,48], the co-volume discretization [37], the mimetic discretization [26] and the edge element [35,36,38].

To determine the band structures of photonic crystals numerically, we need to find the first few branches of positive eigenvalues of the resulting generalized eigenvalue problems

$$\mathbb{A}\vec{\mathbf{e}} = \lambda\mathbb{B}\vec{\mathbf{e}}, \tag{1}$$

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where $\mathbb{A}$ is the matrix corresponding to the discretization of a certain operator and $\mathbb{B}$ is a mass matrix. Furthermore, due to the presence of a large null space associated with (1) [8,12], these target eigenvalues are actually located in the interior of the spectrum of (1). The eigenvalue problem (1) can thus be solved by inverse power method [2,11,12,21], various Lanczos [2,40] or Arnoldi method [4]. These methods use shift-and-invert technique to compute interior eigenpairs and the computational cost for solving the corresponding linear systems can be excessive. On the other hand, we can also use Jacobi–Davidson method [1–4,15,24,41,42] to find the interior target eigenvalues without using the shift-and-invert technique. However, Jacobi–Davidson method still needs to solve linear systems approximately in each of the iterations. In short, the main computational burden is to solve the resulting linear systems (iteratively, as the system is large) within the eigenvalue solvers.

One way to accelerate the processes for solving the linear systems is to find efficient preconditioners. However, it is not a trivial task, especially for three-dimensional photonic band structures. In [12], convergences of the conjugate gradient solver are compared with Jacobi, Successive Over Relaxation (SOR) or Symmetric Successive Over Relaxation (SSOR) preconditioner for computing photonic band structures. For two-dimensional photonic band structures, the SSOR preconditioner can accelerate convergence, while another two preconditioners are ineffective. For the three-dimensional cases, none of the three preconditioners are effective. In [24], a null space free Jacobi–Davidson method are proposed to compute three-dimensional photonic band structures.

To study how we may solve the eigenvalue problems arising in three-dimensional photonic crystals, we first propose using shift-and-invert Krylov–Schur method and Jacobi–Davidson method to solve the generalized eigenvalue problem (1). We then suggest several preconditioning schemes for the associated linear systems. The schemes not only incorporate various common preconditioners like Jacobi, SSOR, ILU (incomplete LU factorization), ICC (incomplete Cholesky factorization). In addition, we derive a preconditioner whose corresponding linear systems can be solved by FFT efficiently. To study the effects of all the preconditioning schemes, we conduct intensive numerical experiments and compare their performance. We find that the combination of the shift-and-invert Krylov–Schur method with the FFT-based preconditioner can be very efficient for solving the target eigenvalue problems.

The paper is organized as follows. The Yee's scheme used to discretize the Maxwell's equations is introduced in Section 1.1. Two particular types of eigenvalue solvers are discussed in Section 2. Several preconditioning schemes are proposed in Section 3. Results of intensive numerical experiments regarding the proposed preconditioning schemes are presented and discussed in Section 4. Finally, we conclude the paper in Section 5.

1.1. Yee's scheme and the model eigenvalue problems

To compute bandgap structures of three-dimensional photonic crystals, we consider the following Maxwell's equations

$$\begin{cases} \nabla \times \boldsymbol{H} = \varepsilon \partial_t \boldsymbol{E}, \\ \nabla \times \boldsymbol{E} = -\mu_0 \partial_t \boldsymbol{H}, \\ \nabla \cdot (\varepsilon \boldsymbol{E}) = 0, \\ \nabla \cdot (\boldsymbol{H}) = 0. \end{cases} \tag{2}$$

By separating the time and space variables and eliminating the magnetic field $\boldsymbol{H}$, the above differential equations become

$$\begin{cases} \nabla \times \nabla \times \boldsymbol{E} = \lambda \varepsilon \boldsymbol{E}, \\ \nabla \cdot (\varepsilon \boldsymbol{E}) = 0 \end{cases} \tag{3}$$

for the electric field $\boldsymbol{E}$, where $\lambda = \mu_0 f^2$ is the unknown eigenvalue, μ_0 and f stands for magnetic constant and frequency, respectively. The permittivity ε is a material dependent constant. Note that the degenerate elliptic operator $\nabla \times \nabla \times$ is self-adjoint and non-negative and (3) is simply an elliptic interface eigenvalue problem.

To solve Eq. (3), we use Yee's scheme to discretize the equation and then derive the resulting generalized eigenvalue problems. Yee's scheme [50] is briefly described here and detailed derivation can be found in, for example, [24,50].

Since the photonic crystals consist of dielectric materials fabricated in periodic structure, Bloch's Theorem [28] suggests that the eigenfunctions of (3) can be written as

$$\boldsymbol{E}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} \boldsymbol{e}(\mathbf{x}), \tag{4}$$

for a vector $\mathbf{k}$ in the first Brillouin zone. The function $\boldsymbol{e}$ satisfies the periodic condition

$$\boldsymbol{e}(\mathbf{x} + \mathbf{a}_\ell) = \boldsymbol{e}(\mathbf{x}) \tag{5}$$

for $\ell = 1, 2, 3$. Here the lattice translation vectors $\mathbf{a}_\ell$ span the primitive cell which extends periodically to form the photonic crystal. Now, we can rewrite Eq. (3) as

$$e^{-i\mathbf{k}\cdot\mathbf{x}} \nabla \times \nabla \times e^{i\mathbf{k}\cdot\mathbf{x}} \boldsymbol{e} = \lambda \varepsilon \boldsymbol{e}. \tag{6}$$

Letting

$$\boldsymbol{h} = \nabla \times e^{i\mathbf{k}\cdot\mathbf{x}} \boldsymbol{e} \tag{7}$$