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Parallel two-level domain decomposition based Jacobi–Davidson algorithms for pyramidal quantum dot simulation

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ABSTRACT

We consider a quintic polynomial eigenvalue problem arising from the finite volume discretization of a quantum dot simulation problem. The problem is solved by the Jacobi–Davidson (JD) algorithm. Our focus is on how to achieve the quadratic convergence of JD in a way that is not only efficient but also scalable when the number of processor cores is large. For this purpose, we develop a projected two-level Schwarz preconditioned JD algorithm that exploits multilevel domain decomposition techniques. The pyramidal quantum dot calculation is carefully studied to illustrate the efficiency of the proposed method. Numerical experiments confirm that the proposed method has a good scalability for problems with hundreds of millions of unknowns on a parallel computer with more than 10,000 processor cores.

1. Introduction

Polynomial eigenvalue problems are of great interest because there are many important applications in science and engineering, such as the stability analysis in fluid mechanics, the vibration problem in solid mechanics, the quantum dot problem in nanotechnology; see [1–7] and references therein. The JD algorithm, originally proposed by Sleijpen and Van der Vorst for solving algebraic linear eigenvalue problems [8,9], has been shown to be effective for polynomial eigenvalue problems [1,2,10,11], especially for the case when several interior eigenvalues are of interest. The JD algorithm belongs to a class of subspace iterative methods, which consists of two key steps: first increase the search space by adding a new basis vector and then extract the approximate eigenpair from the search space through a Rayleigh–Ritz procedure. To obtain a new basis vector for the search space, at each JD iteration, one needs to solve inexactly a large sparse linear system of equations, which is referred to as the correction equation, by a preconditioned Krylov subspace type method, such as GMRES or CG methods [12].

The numerical experiences suggest that the robustness and the efficiency of the JD algorithm depend on the following three factors: (1) the initial search space, (2) the Ritz pair selection strategy, and (3) the solution quality of the correction equation. Similar to Newton-type methods for solving nonlinear systems, the JD algorithm is a locally convergent iterative method, i.e., if the initial guess is not close enough to the exact solution, the convergence often exhibits some stagnation behavior, or even worse, is not achieved. One important feature of the JD algorithm is that at each JD iteration, only mild solution accuracy of the correction equation is required. Several recent publications were related to the correction equation solvers. Feng [6] applied a multilevel JD method for the generalized eigenvalue problem with application in the finite element analysis of structural dynamic problems. A multigrid-type preconditioner was used in conjugation with FGMRES as the correction equation solver. The incomplete Cholesky factorization without fill-ins was employed as the pre- and post-smoothers and the coarse grid problem was solved by a direct method. Arbenz et al. [5] proposed a hybrid preconditioner combining a hierarchical basis preconditioner and an algebraic multigrid preconditioner for the correction equation in the JD algorithm for solving symmetric generalized Maxwell eigenvalue problem; they reported good parallel scalability using up to 16 processors.

The aim of the paper is to develop and study a two-level JD algorithm for the large sparse polynomial PDE eigenvalue problems and its applications in quantum dot simulations. The concept of two-level approach fits in the JD algorithm in three aspects. The first idea is to use a coarse mesh to construct the

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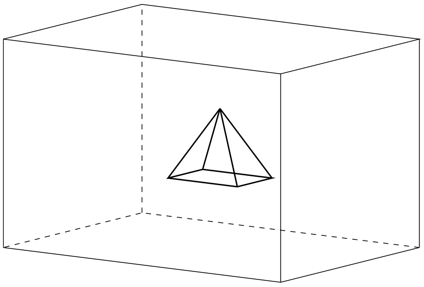

Fig. 1. Structure of a pyramidal quantum dot embedded in a cuboid.

initial vector in the search space since for many applications, the smooth eigenvector corresponding to the low frequency can be well represented by the coarse mesh solution. The second idea is to use the coarse solution as a guideline for selecting a proper Ritz-pair. For example [2], a similarity measure was applied using the coarse eigenvalues and eigenvectors as a reference to avoid picking un-physical spurious root introduced during the Raleigh–Ritz projection procedure. The third idea is in the construction of the preconditioner using the domain decomposition method for the Krylov subspace iterative-type correction equation solver. Our proposed two-level preconditioner is based on the Schwarz framework [13–15], which has a long successful history for linear elliptic PDEs. We also compare numerically the proposed approach with a one-level method, and a popular two-level orthogonal Arnoldi (TOAR) method using PETSc [16] and SLEPc [17]. Our approach outperforms both of them in terms of the total compute time, and the strong scalability on a machine with a large number of processor cores.

The rest of the paper is organized as follows. Section 2 briefly introduces the pyramidal quantum dot problem. In Section 3, we propose a projected two-level domain decomposition based Jacobi–Davidson algorithm. Numerical results of the proposed algorithm and comparison with other methods are reported in Section 4. Some final remarks are given in Section 5.

2. Pyramidal quantum dot problem

We consider polynomial eigenvalue problems arising from quantum dot (QD) simulations. An example of QD is a pyramid dot embedded in a cuboid as shown in Fig. 1. Due to the confinement effect, the pyramidal quantum dot has discrete energy states. This type of quantum dot can be produced by a few manufacturing procedures and has many applications, such as lasers and single-electron devices [18].

The central task is to compute some energy states and their corresponding wave functions, by solving an eigenvalue problem [1,3,4,18–22]. The quantum states of a pyramidal quantum dot with a single electron can be described by the time-independent 3D Schrödinger equation

$$-\nabla\cdot\left(\frac{\hbar^2}{2m(\mathbf{r},\lambda)}\nabla u\right)+V(\mathbf{r})u=\lambda u, \qquad (1)$$

on the domain Ω, where λ is called an energy state or eigenvalue, and u is the corresponding wave function or eigenvector. In (1), $\hbar$ is the reduced Planck constant, $\mathbf{r}$ is the space variable, $m(\mathbf{r},\lambda)$ is the effective electron mass, and $V(\mathbf{r})$ is the confinement potential. Taking the effect of the spin–orbit splitting into account, the effective mass model

$$m(\mathbf{r},\lambda)=\begin{cases}m_1(\lambda) & \text{in the pyramid}\\ m_2(\lambda) & \text{in the cuboid}\end{cases}$$

$$V(\mathbf{r})=\begin{cases}V_1 & \text{in the pyramid}\\ V_2 & \text{in the cuboid}\end{cases}$$

can be derived from the eight-band $\mathbf{k}\cdot\mathbf{p}$ analysis and the effective mass theory [3,22]. More precisely,

$$\frac{1}{m_i(\lambda)}=\frac{P_i^2}{\hbar^2}\left(\frac{2}{\lambda+\ell_i-V_i}+\frac{1}{\lambda+\ell_i-V_i+\delta_i}\right), \quad i=1,2, \qquad (2)$$

where P_i, ℓ_i and δ_i are the momentum, main energy gap and spin–orbit splitting corresponding to the pyramid and the cuboid, respectively.

Since the pyramidal QD is a heterostructure, the Ben Daniel–Duke condition [1,3] is imposed on the interface of the two materials:

$$\left.\left(\frac{1}{m(\mathbf{r},\lambda)}\frac{\partial u}{\partial \mathbf{n}}\right)\right|_{\partial D_-}=\left.\left(\frac{1}{m(\mathbf{r},\lambda)}\frac{\partial u}{\partial \mathbf{n}}\right)\right|_{\partial D_+} \qquad (3)$$

where D denotes the domain of the pyramid dot and $\mathbf{n}$ is the unit outward normal for each surface of ∂D. Since the corresponding wave functions decay exponentially outside the pyramid dot, the homogeneous Dirichlet boundary condition

$$u=0 \qquad (4)$$

is imposed on the boundary of the cuboid $\partial\Omega$.

A cell-centered second-order finite volume method [3] on a uniform mesh in Cartesian coordinates is applied to discretize the Schrödinger equation with non-parabolic effective mass model. With this finite volume method, the interface condition (3) is applied implicitly. The resulting system is a polynomial eigenvalue problem

$$(\lambda^5A_5+\lambda^4A_4+\lambda^3A_3+\lambda^2A_2+\lambda A_1+A_0)x=0, \qquad (5)$$

where $\lambda\in\mathbb{C}$, $x\in\mathbb{C}^N$, $A_i\in\mathbb{R}^{N\times N}$, and N is the total number of unknowns. The matrices A_5 and A_4 are diagonal, and all other matrices are nonsymmetric.

3. Jacobi–Davidson algorithm with a projected two-level Schwarz preconditioner for the correction equation

We begin with some notations. For given $A_i\in\mathbb{C}^{N\times N}$, $i=0,1,\ldots,m$, such that their null spaces only have a trivial intersection, we define

$$\mathcal{A}_\phi=\sum_{i=0}^{m}\phi^iA_i$$

as a matrix polynomial of $\phi\in\mathbb{C}$. If there exist $\lambda\in\mathbb{C}$ and nonzero $x\in\mathbb{C}^N$ such that

$$\mathcal{A}_\lambda x=0, \qquad (6)$$

then λ is called an eigenvalue of $\mathcal{A}_\phi$ and x is the right eigenvector of $\mathcal{A}_\phi$ associated with the eigenvalue λ. In general, (6) is referred to as the polynomial eigenvalue problem of degree m.

The Jacobi–Davidson algorithm is a powerful approach for solving the polynomial eigenvalue problem (6). The details of the JD algorithm are summarized in Algorithm 1. Since the correction equation is the most expensive part of computation, the parallel performance of the JD algorithm is determined mostly by how the correction equation is solved. We introduce a projected two-level Schwarz preconditioner that improves greatly the convergence of the correction equation solver and is scalable.

In Algorithm 1, Step 3 implies a Galerkin condition that r is orthogonal to the subspace *span*$\{V\}$. At each JD iteration, the projected polynomial eigenproblem is solved by the QZ method with linearization, see [1,17] for details. Then ϕ is chosen to be the desired eigenvalue that is closest to the initial guess eigenvalue θ, that is, $|\phi-\theta|$ is minimum among all the eigenvalues of the projected polynomial eigenproblem. If the accuracy of (ϕ,u) is