Parallel performance of CIRR method with complete factorization preconditioner on multi-core

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Abstract. We consider a parallel method for solving generalized eigenvalue problems that arise from molecular orbital calculation of the biochemistry application. Our focus is to develop scalable parallel implementations of the method that achieves high performance on multi-core clusters. In a Rayleigh-Ritz type method using a contour integral (CIRR method), the computation at each contour involves linear system solutions. We apply a Krylov subspace iterative method with a complete factorization preconditioner. We report parallel performance of our method on multi-core processors.

Key words: Parallel eigenvalue solver, complete factorization preconditioner, interior eigenvalue problem

1 Introduction

We consider a method for solving generalized eigenvalue problems that arise from molecular orbital calculation of the biochemistry application. The prediction of the electron distribution requires a set of multiple eigenpairs the generalized eigenvalue problem

$$A\boldsymbol{x} = \lambda B\boldsymbol{x},$$

where $A \in \mathbb{R}^{n\times n}$ is symmetric, and $B \in \mathbb{R}^{n\times n}$ is symmetric positive definite. Each eigenvalue problem represents a certain part of a physical domain. Our focus is to develop scalable parallel implementations of the method that provides high performance on multi-core clusters.

The method for finding eigenpairs in a given physical domain is based on contour integral presented in [3]. The major advantage of this method is that it is very suitable for master-worker programming models because iterative process for constructing subspaces is not required. We recently proposed a Rayleigh-Ritz

type method [6] and a block variant [1] of the method in order to improve numerical stability. The computation at each contour involves linear system solutions where the coefficient matrices are derived from A and B. In [2], we found that a Krylov subspace iterative method in conjunction with a preconditioning using a complete factorization for an approximated coefficient matrix is effective to solve such linear systems.

In our eigenvalue solver, a projected matrix pencil with eigenvalues of interest are derived by solution of linear systems. Therefore, if multiple eigenvalues in certain physical domains are required, corresponding linear systems need to be solved. Those systems can be solved independently, allowing a variety of parallel programming model. Our first parallel implementation of the eigenvalue solver based on a GridRPC [4, 5] executes a sequential linear system solver for each of linear systems deployed to a single node of PC clusters. We extend this discussion to the performance of our eigenvalue solver on PC cluster of multicore processors. In particular, we focus on the performance on preconditioned iterative solvers.

2 A Rayleigh-Ritz type method with a contour integral

In this section, we show an eigenvalue solver using contour integral presented in [6]. Let $(\lambda_j, \boldsymbol{x}_j)$, $1 \leq j \leq n$ be eigenpairs of the matrix pencil (A, B). Suppose that m distinct eigenvalues $\lambda_1, \ldots, \lambda_m$ are located inside a positively oriented closed Jordan curve Γ in $\mathbb{C}$.

For a nonzero vector $\boldsymbol{v} \in \mathbb{R}^n$, we define

$$\boldsymbol{s}_k := \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} (z-\gamma)^k (zB-A)^{-1} B\boldsymbol{v} \, \mathrm{d}z, \quad k = 0, 1, \ldots, m-1, \tag{1}$$

where $\gamma \in \mathbb{R}$ is located inside Γ. Let $S := [\boldsymbol{s}_0, \ldots, \boldsymbol{s}_{m-1}]$, and let $Q := [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m]$ be orthonormal basis obtained from S. Then we have the following theorem([6]).

Theorem 1. *If $\lambda_1, \ldots, \lambda_m$ are distinct and $\boldsymbol{v}^T B \boldsymbol{x_j} \neq 0$ for $1 \leq j \leq m$ then*

$$\mathrm{span}\{\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m\} = \mathrm{span}\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}. \tag{2}$$

This theorem implies that the Galerkin approximation to the matrix pencil (A, B) on the subspace spanned by $[\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m]$ provides the exact eigenpairs $(\lambda_j, \boldsymbol{x}_j)$, $1 \leq j \leq m$. We apply a Rayleigh-Ritz procedure with the projected matrices given by $\tilde{A} = Q^{\mathrm{T}} A Q$ and $\tilde{B} = Q^{\mathrm{T}} B Q$. The Ritz values of the projected pencil $(\tilde{A}, \tilde{B})$ are eigenvalues of the original pencil (A, B) in Γ and Ritz vectors are corresponding eigenvectors.

When Γ is a circle with the center γ and the radius ρ, the integral (1) is approximated via the N-point trapezoidal rule:

$$\hat{\boldsymbol{s}}_k = \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} (\omega_j B - A)^{-1} B\boldsymbol{v}, \quad k = 0, 1, \ldots m-1, \tag{3}$$

where $\omega_j = \gamma + \rho \exp(2\pi \mathrm{i} j/N + 1/2)$ and N is a positive integer. In these computations, we solve the systems of linear equations

$$(\omega_j B - A)\boldsymbol{y}_j = B\boldsymbol{v}, \quad j = 0, 1, \ldots, N-1. \tag{4}$$

Note that the solutions $\boldsymbol{y}_j$, $N/2 \leq j \leq N-1$ are obtained from the relation $\boldsymbol{y}_j = \bar{\boldsymbol{y}}_{N-j-1}$. Thus we only need to solve $N/2$ systems.

A block variant of the method is proposed in [1], which improves numerical accuracy. In this method, a matrix $V := [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L] \in \mathbb{R}^{n \times L}$ is used instead of $\boldsymbol{v}$ in (4), where $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_L$ are linearly independent, and positive integer L is a block size. Then the numerical integration (3) is replaced as

$$\hat{S}_k = \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} (\omega_j B - A)^{-1} BV \quad k = 0, 1, \ldots, M-1, \tag{5}$$

with systems of linear equations

$$(\omega_j B - A)Y_j = BV, \quad j = 0, 1, \ldots, N-1, \tag{6}$$

where M is a positive integer which is chosen so that $M \geq m/L$. Set $\hat{S} = [\hat{S}_0, \ldots, \hat{S}_{M-1}]$, and we obtain a matrix S' which is constructed from the first m' column vectors of $\hat{S}$, where m' is chosen so that S' is nonsingular. The algorithm of the block variant of the CIRR method is as follows:

Algorithm (Block CIRR method)

Input: $V \in \mathbb{R}^{n \times L}$, M, N, γ, ρ

Output: $(\hat{\lambda}_j, \hat{\boldsymbol{x}}_j)$, $1 \leq j \leq m'$

1. Set $\omega_j = \gamma + \rho \exp(2\pi \mathrm{i}(j + 1/2)/N)$, $j = 0, \ldots, N-1$.
2. Solve $(\omega_j B - A)Y_j = BV$ for Y_j, $j = 0, \ldots, N-1$.
3. Compute $\hat{S}_k$, $k = 0, \ldots, M-1$.
4. Set m' using the singular value decomposition of $\hat{S} = [\hat{S}_0, \ldots, \hat{S}_{M-1}]$, and set $S' = \hat{S}(:, 1 : m')$.
5. Construct an orthonormal basis Q from S'.
6. Form $\tilde{A} = Q^{\mathrm{T}} A Q$ and $\tilde{B} = Q^{\mathrm{T}} B Q$.
7. Compute the Ritz pairs $(\hat{\lambda}_j, \hat{\boldsymbol{x}}_j)$, $1 \leq j \leq m'$ of the projected pencil $(\tilde{A}, \tilde{B})$.

3 A preconditioner using a complete factorization

When matrices A and B are large, the computational costs for solving systems of linear equations (6) are dominant in the method. In our application, matrices have relatively large number of nonzero elements due to the base function of middle-range interaction of molecules. We apply a Krylov subspace iterative method with a complete factorization preconditioner presented in [2].

In this preconditioner, a complete factorization of the approximate matrix $\hat{C}_j$ for the coefficient matrix $C_j := \omega_j B - A$ is used. The approximate matrix $\hat{C}_j$ is obtained from drop-thresholding of the original coefficient matrix C_j. Due to less nonzero entries in $\hat{C}_j$ than C_j, we expect fewer nonzeroes in the preconditioner than the matrix factor obtained from factorization of C_j. The drop-thresholding is defined as follows:

$$|c_{ij}| \leq \max_{1 \leq k,l \leq n} (|c_{kl}|) \times \alpha \Rightarrow c_{ij} = 0,$$

where α is a small positive number.

Since systems (6) can be solved independently for j, we solve $N/2$ systems

$$C_j Y_j = BV, \quad j = 0, 1, \ldots, N/2 - 1$$

on each node of clusters. Before starting the iterative process of the Krylov subspace method, the approximate matrix $\hat{C}_j$ is factorized, and then back-substitutions and matrix-vector products are performed in the iterative process. These three parts are dominant in computational costs to solve the system. We will report parallel performance of our method on multi-core processors.

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