A PARALLEL-IN-TIME PRECONDITIONER FOR THE SCHUR COMPLEMENT OF PARABOLIC OPTIMAL CONTROL PROBLEMS

XUELIE LIN*, SHU-LIN WU†, AND ZHIMING ZHANG‡

Abstract. For optimal control problems constrained by an initial-valued parabolic PDE, we have to solve a large scale saddle point algebraic system consisting of considering the discrete space and time points all together. A popular strategy to handle such a system is the Krylov subspace method, for which an efficient preconditioner plays a crucial role. The matching-Schur-complement preconditioner has been extensively studied in literature and the implementation of this preconditioner lies in solving the underlying PDEs twice, sequentially in time. In this paper, we propose a new preconditioner for the Schur complement, which can be used parallel-in-time (PinT) via the so-called diagonalization technique. We show that the eigenvalues of the preconditioned matrix are low and upper bounded by positive constants independent of matrix size and the regularization parameter. The uniform boundedness of the eigenvalues leads to an optimal linear convergence rate of conjugate gradient solver for the preconditioned Schur complement system. To the best of our knowledge, it is the first time to have an optimal convergence analysis for a PinT preconditioning technique of the optimal control problem. Numerical results are reported to show that the performance of the proposed preconditioner is robust with respect to the discretization step-sizes and the regularization parameter.

Key words. parallel-in-time (PinT), diagonalization, Schur complement preconditioner, parabolic optimal control, optimal convergence rate

1. Introduction. We consider the optimal control problem:

$$\min_{y,u} \mathcal{L}(y,u) := \frac{1}{2} \left| y - g \right|_{L^2(\Omega \times (0,T))}^2 + \frac{\gamma}{2} \left| u \right|_{L^2(\Omega \times (0,T))}^2,$$  

subject to a linear parabolic equation with initial- and boundary-value conditions

$$\begin{cases}
y_t - Ly = f + u, & \text{in } \Omega \times (0,T), \\
y = 0, & \text{on } \partial \Omega \times (0,T), \\
y(\cdot,0) = y_0, & \Omega,
\end{cases}$$

where $g$, $f$, $y_0$ are all given functions and $\gamma > 0$ is a given regularization parameter that is supposed to be small. The space operator $\mathcal{L}$ considered here is the diffusion operator $\mathcal{L} = \nabla(a(x)\nabla \cdot)$ with $a(x) \geq 0$, but other self-adjoint operators can be also included.

The optimal control problem with parabolic PDE constraint is a class of important problem that has attracted intensive consideration and studies, due to its various applications in real world; see ???. Analytical solutions of optimal control problems are typically unavailable. Because of this, numerical methods for parabolic PDE-constrained optimal control problems have been widely studied; see, e.g., [5–7, 10].

Following an optimize-then-discretize approach and by applying the first-order optimality condition, we get the following KKT system (see, e.g., [1, 3] for more details):

$$\begin{bmatrix} I & 0 & L \gamma I \\
0 & I & -I \\
L & -I & 0 \end{bmatrix} \begin{bmatrix} y \\
u \\
p \end{bmatrix} = \begin{bmatrix} g \\
0 \\
f \end{bmatrix},$$

*Shenzhen JL Computational Science and Applied Research Institute, Shenzhen, 518131 China. E-mail: linxuelei@csar.ac.cn
†The corresponding author, School of Mathematics and Statistics, Northeast Normal University, Changchun 130024, China. E-mail: wushulin84@hotmail.com
‡Beijing Computational Science Research Center, Beijing 100193, China; and Department of Mathematics, Wayne State University, Detroit, MI 48202, USA. E-mails: zmzhang@csrc.ac.cn and ag7761@wayne.edu.
where \( p \) is the Lagrange multiplier; \( \mathcal{L}_1 \) and \( \mathcal{L}_2 \) are defined by
\[
\mathcal{L}_1 y := (\partial_t - \mathcal{L})y, \quad \text{with } y(x, 0) = y_0(x),
\]
\[
\mathcal{L}_2 p := (-\partial_t - \mathcal{L})p, \quad \text{with } p(x, T) = 0.
\]
Here, \( y \) evolves forward from \( t = 0 \) to \( t = T \) and \( p \) evolves backward from \( t = T \) to \( t = 0 \). By eliminating the control variable \( u \), the KKT system is reduced to
\[
\begin{bmatrix}
    I & \mathcal{L}_2 \\
    \mathcal{L}_1 & -\gamma^{-1}I
\end{bmatrix}
\begin{bmatrix}
y \\
p
\end{bmatrix} =
\begin{bmatrix}
y \\
f
\end{bmatrix}
\tag{1.2}
\]

For space discretization of (1.2), we suppose that the Laplacian operator \( \mathcal{L} \) is approximated by a symmetric positive semi-definite matrix \( \mathcal{L}_h \), i.e., \( \mathcal{L} \approx \mathcal{L}_h \) by any scheme (e.g., the finite difference method or the finite element method). For time discretization, we consider the Trapezoidal rule which is a second-order time-integrator. The resulting discrete KKT system is
\[
\begin{bmatrix}
    \frac{2}{\tau}B_2 \otimes I_x & B_1^T \otimes I_x + \frac{2}{\tau^2}B_2^T \otimes \mathcal{L}_h \\
    B_1 \otimes I_x + \frac{2}{\tau}B_2 \otimes \mathcal{L}_h & -\frac{2}{\tau^2}B_2 \otimes I_x
\end{bmatrix}
\begin{bmatrix}
y_{\tau,h} \\
p_{\tau,h}
\end{bmatrix} =
\begin{bmatrix}
g_{\tau,h} \\
f_{\tau,h}
\end{bmatrix},
\tag{1.3}
\]
where \( I_x \in \mathbb{R}^{J \times J} \) is identity matrix with \( J \) being the number of spatial grids and \( N = T/\tau \) is the number of discrete time points with \( \tau \) being the time step size. The two matrices \( B_1 \) and \( B_2 \) are
\[
B_1 = \begin{bmatrix}
1 & 1 & \cdots & 1 \\
-1 & 1 & \cdots & 1 \\
\vdots & \ddots & \ddots & \vdots \\
-1 & \cdots & \cdots & 1
\end{bmatrix}, \quad B_2 = \begin{bmatrix}
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \ddots & \ddots & \vdots \\
1 & \cdots & \cdots & 1
\end{bmatrix} \in \mathbb{R}^{N \times N}.
\]
The symbol ‘\( \otimes \)’ denotes the Kronecker product. We note that the Schur complement of (1.3) is non-symmetric, which is due to the asymmetry of \( B_2 \). If the backward-Euler method (considered by many works in the literature) is employed to discretize \( \partial_t \), then the resulting discrete KKT system is still of form (1.3) but with \( B_2 \) replaced by a scaled identity matrix; and in such case, the Schur complement is symmetric-positive definite and thus easier to invert. So, the usage of high-order scheme (Trapezoidal rule) has its price compared with the low-order scheme (backward-Euler method), as the \( B_2 \) brought by the Trapezoidal rule has a more complicated structure than the scaled identity matrix from the backward-Euler method. To make the Schur complement of KKT system arising from Trapezoidal rule symmetric, we consider applying a block-diagonal scaling to (1.3):
\[
\begin{bmatrix}
\frac{2}{\tau}B_2 \otimes I_x & B_1^T \otimes I_x + \frac{2}{\tau^2}B_2^T \otimes \mathcal{L}_h \\
B_1 \otimes I_x + \frac{2}{\tau}B_2 \otimes \mathcal{L}_h & -\frac{2}{\tau^2}B_2 \otimes I_x
\end{bmatrix}
\begin{bmatrix}
y_{\tau,h} \\
p_{\tau,h}
\end{bmatrix} =
\begin{bmatrix}
g_{\tau,h} \\
f_{\tau,h}
\end{bmatrix},
\tag{1.4}
\]
where \( W = \text{blockdiag}(B_2 \otimes I_x, B_2^T \otimes I_x) \). It is straightforward to verify that
\[
B_2^{-1} = \begin{bmatrix}
s_0 & s_0 & \cdots & s_0 \\
s_1 & s_0 & \cdots & s_0 \\
\vdots & \ddots & \ddots & \vdots \\
s_{N-1} & \cdots & s_1 & s_0
\end{bmatrix}, \quad s_k = (-1)^k, \quad k = 0, 1, \ldots, N - 1,
\tag{1.6}
\]
\[
B_1B_2^{-1} = B_2^{-1}B_1 = \begin{bmatrix}
q_0 & q_0 & \cdots & q_0 \\
q_1 & q_0 & \cdots & q_0 \\
\vdots & \ddots & \ddots & \vdots \\
q_{N-1} & \cdots & q_1 & q_0
\end{bmatrix}, \quad q_0 = 1, \quad q_k = 2(-1)^k, \quad k \geq 1. \tag{1.7}
\]
(1.6) and (1.7) show that $B_2^{-1}$ and $B_3^{-1} B_1$ are both Toeplitz matrix; and that $B_1$ and $B_2^{-1}$ are commutative. Since $W^{-1} = \text{blockdiag}(B_2^{-1} \otimes I_x, B_2^{-1} \otimes I_x)$ and $B_2^{-1}$ has a simple expression as shown in (1.6), it is trivial to compute $p_{r,h}$ and $y_{r,h}$ from (1.5) once $\tilde{y}_{r,h}$ and $\tilde{p}_{r,h}$ are computed. Hence, it remains to solve the linear system (1.4).

Denote $B = B_2^{-1} B_1$.

Then, the commutativity between $B_1$ and $B_2^{-1}$ imply that

$$W^{-1} = \begin{bmatrix}
\frac{1}{2} B_2 \otimes I_x & B_1^T \otimes I_x + \frac{1}{2} B_2^T \otimes \mathcal{L}_h \\
B_1 \otimes I_x + \frac{1}{2} B_2 \otimes \mathcal{L}_h & -\frac{1}{2} B_2^T \otimes I_x \\
\frac{1}{2} I_t \otimes I_x & B^T \otimes I_x + \frac{1}{2} I_t \otimes \mathcal{L}_h \\
B \otimes I_x + \frac{1}{2} I_t \otimes \mathcal{L}_h & -\frac{1}{2} I_t^T \otimes I_x
\end{bmatrix},$$

where $I_t \in \mathbb{R}^{N \times N}$ denotes the $N \times N$ identity matrix. Hence, (1.4) can be rewritten as

$$\begin{bmatrix}
\frac{1}{2} I_t \otimes I_x & B^T \otimes I_x + \frac{1}{2} I_t \otimes \mathcal{L}_h \\
B \otimes I_x + \frac{1}{2} I_t \otimes \mathcal{L}_h & -\frac{1}{2} I_t^T \otimes I_x
\end{bmatrix} \begin{bmatrix}
\tilde{y}_{r,h} \\
\tilde{p}_{r,h}
\end{bmatrix} = \begin{bmatrix}
g_{r,h} \\
\tau h_f
\end{bmatrix}.$$ (1.8)

Unlike (1.3), the Schur complement of (1.8) is symmetric positive-definite (by multiplying $-1$) and thus efficient preconditioned conjugate gradient (PCG) solver is applicable and analyzable. This is the purpose of applying the block diagonal scaling in (1.4).

Preconditioning techniques for discrete KKT system arising from optimal control problem is reviewed as follows. In [9], a regularization-robust preconditioner is proposed for Schur complement of the KKT system, with which the eigenvalues of the preconditioned matrix are proven to be lower bounded by 0.5 and upper bounded by 1. Nevertheless, the regularization-robust preconditioner proposed in [9] is not implemented in a PinT manner, since its inversion requires to solve two discrete time-dependent PDEs one time-step by one time-step. In [11], a diagonalization-based preconditioner is proposed for the KKT system, which can be implemented in a PinT manner. Although the numerical results in [11] show that the diagonalization-based preconditioner is efficient, there is no theoretical result provided on the bounds of the spectrum of the preconditioned matrix.

In this paper, we propose a block-circulant-based preconditioner $\mathcal{P}_\epsilon$ for a scaled Schur complement $\mathcal{K}$ (defined in (2.4)) of the KKT matrix in (1.8), where $\epsilon \in (0, 1)$ is a free parameter. The proposed preconditioner $\mathcal{P}_\epsilon$ is a product of two matrices that are diagonalizable in temporal dimension, because of which the inversion of $\mathcal{P}_\epsilon$ can be implemented in a PinT manner. This is why we call $\mathcal{P}_\epsilon$ a PinT preconditioner. Since both $\mathcal{P}_\epsilon$ and $\mathcal{K}$ are symmetric positive-definite, the PCG solver is applicable to the preconditioned system. Theoretically, we show that the spectrum of the preconditioned matrix lies in $[\frac{3}{4}, \frac{5}{4}]$ provided that $\epsilon \leq C \tau^2 \gamma^{-1/2}$ with a moderate quantity $C$. Because of this uniformly bounded spectrum, the convergence factor of each PCG iteration is always smaller than 1/3 as shown in Theorem 3.10. Such a convergence factor is independent of matrix-size parameters $N, J$, and the regularization parameter $\gamma$. That means the complexity of PCG solver is proportional to the complexity of a matrix-vector multiplication of the preconditioned matrix, which is optimal. This is why we call the matrix-size independent convergence rate as the optimal convergence rate. Numerical results show that the PCG solver for the preconditioned system converges even faster than the theoretical result predict.

The contribution of this paper is twofold. First, a preconditioner $\mathcal{P}_\epsilon$ that can be implemented in a PinT manner is proposed for the optimal control problem so that the
process of solving the optimal control problem is PinT. Second, we can show theoretically that the PCG solver for the preconditioned system has an optimal convergence rate independent of matrix size and regularization parameter. To the best of our knowledge, it is the first time to have an optimal convergence theoretical guarantee for a PinT preconditioner of the optimal control problem.

The rest of this paper is structured as follows. In Section 2, the Schur complement system, the PinT preconditioner and its implementation are presented. In Section 3, the spectrum of the preconditioned matrix and optimal convergence of PCG solver for the preconditioned system are analyzed. In Section 4, numerical results are presented to show the performance of the proposed preconditioning technique. Finally, concluding remarks are given in Section 5.

2. The Schur Complement of (1.8) and the Proposed PinT Preconditioner. In this section, we present the Schur complement system corresponding to (1.8) and introduce our PinT preconditioner for the Schur complement system.

**Lemma 2.1.** If both $A_1$ and the Schur complement $A_4 - A_3A_1^{-1}A_2$ are invertible, the inverse of a $2 \times 2$ block matrix can be expressed as follows

$$
\begin{bmatrix}
A_1 & A_2 \\
A_3 & A_4 \\
\end{bmatrix}^{-1} = \begin{bmatrix}
I & -A_1^{-1}A_2 \\
-A_3A_1^{-1}A_2 & I \\
\end{bmatrix} \begin{bmatrix}
A_1^{-1} & 0 \\
0 & (A_4 - A_3A_1^{-1}A_2)^{-1} \\
\end{bmatrix} \begin{bmatrix}
I \\
-A_3A_1^{-1} \\
\end{bmatrix}.
$$

Applying Lemma 2.1 to (1.8) yields

$$
\begin{bmatrix}
\tilde{y}_{\tau,h} \\
\tilde{p}_{\tau,h} \\
\end{bmatrix} = \begin{bmatrix}
I & \frac{G}{\tau} \\
\frac{2}{\tau}I_t \otimes I_x & -2\gamma(\tau I_t \otimes I_x + \eta GG^T)^{-1} \\
\end{bmatrix} \begin{bmatrix}
I \\
\frac{G}{\tau} \\
\end{bmatrix} \begin{bmatrix}
g_{\tau,h} \\
f_{\tau,h} \\
\end{bmatrix},
$$

where $I$ denotes the $(NJ) \times (NJ)$ identity matrix.

$$
\eta = \frac{\gamma}{\tau}, \quad G = 2B \otimes I_x + \tau I_t \otimes L_h.
$$

Clearly, the most heavy computational burden is to solve the following Schur complement linear system

$$
\mathcal{K}v = b,
$$

where $b \in \mathbb{R}^{NJ \times 1}$ is some given vector;

$$
\mathcal{K} = \tau I_t \otimes I_x + \eta GG^T.
$$

A routine calculation yields

$$
\mathcal{K} = (\tau I_t + 4\eta BB^T) \otimes I_x + 2\eta(B + B^T) \otimes L_h + \tau^2 \eta I_t \otimes L_h^2.
$$

To construct the preconditioner for $\mathcal{K}$, we firstly introduce an intermediate approximation $\mathcal{P}$ to $\mathcal{K}$. Denote

$$
\mathcal{P} := \mathcal{R}\mathcal{R}^T,
$$

where

$$
\mathcal{R} = (\sqrt{\tau}I_t + 2\sqrt{\eta}B) \otimes I_x + \tau \sqrt{\eta}I_t \otimes L_h.
$$

Note that the inversion of $\mathcal{P}$ requires the inversion of $\mathcal{R}$ and $\mathcal{R}^T$. However, $\mathcal{R}$ ($\mathcal{R}^T$) has block lower (upper) triangular structure. The inversion of block lower (upper) triangular matrix involves block forward (backward) substitution algorithm, which is not PinT. Hence, we do not intend to use $\mathcal{P}$ as a preconditioner directly. Instead, we use an approximation $\mathcal{P}_\epsilon$ to $\mathcal{P}$ as a preconditioner for $\mathcal{K}$, which is defined as follows.

$$
\mathcal{P}_\epsilon = \mathcal{R}_\epsilon \mathcal{R}_\epsilon^T,
$$

(2.8)
Here, we recall that the above numbers \( q_i \)'s are defined in (1.7). We will prove the invertibility of \( \mathcal{R}_\epsilon \) and thus the invertibility of \( \mathcal{P}_\epsilon \) for some properly chosen \( \epsilon \) in the next section. From the definition of \( \mathcal{P}_\epsilon \), it is clear that \( \mathcal{P}_\epsilon \) is a symmetric positive definite matrix. Instead of solving (2.3) directly, we apply preconditioned conjugate gradient (PCG) solver to solve the following preconditioned system

\[
\mathcal{P}_\epsilon^{-1} \mathbf{K} \mathbf{v} = \mathcal{P}_\epsilon^{-1} \mathbf{b}.
\]  

(2.11)

In each PCG iteration, we need to compute some matrix vector products \( \mathcal{P}_\epsilon^{-1} \mathbf{K} \mathbf{w} \) for some given vector \( \mathbf{w} \in \mathbb{R}^{N J} \). One can compute the product \( \mathbf{K} \mathbf{w} \) first and then compute the product \( \mathcal{P}_\epsilon^{-1} (\mathbf{K} \mathbf{w}) \) once \( \mathbf{K} \mathbf{w} \) is computed. As \( \mathbf{K} \) is sparse matrix, the computation of the product \( \mathbf{K} \mathbf{w} \) requires \( O(NJ) \) flops. Hence, we only need to consider the computation of \( \mathcal{P}_\epsilon^{-1} \mathbf{w} \) for a given vector \( \mathbf{w} \). From \( \mathcal{P}_\epsilon^{-1} = \mathcal{R}_\epsilon^{-1} \mathcal{R}_\epsilon^{-T} \), we know that \( \mathcal{P}_\epsilon^{-1} \mathbf{w} \) can be computed by \( \mathcal{P}_\epsilon^{-1} \mathbf{w} = \mathcal{R}_\epsilon^{-1} (\mathcal{R}_\epsilon^{-T} \mathbf{w}) \). Hence, to fast implement the matrix-vector product of \( \mathcal{P}_\epsilon^{-1} \), it suffices to fast implement the matrix-vector products corresponding to \( \mathcal{R}_\epsilon^{-1} \) and \( \mathcal{R}_\epsilon^{-T} \). We firstly discuss a fast PinT implementation for computing the product between \( \mathcal{R}_\epsilon^{-1} \) and an arbitrarily given vector \( \mathbf{r} \).

Actually, \( \mathcal{B}_\epsilon \) is diagonalizable by means of Fourier transform (see, [4]). The diagonalization formula is shown as follows.

\[
\mathcal{B}_\epsilon = \mathcal{D}_\epsilon^{-1} \mathcal{F}_N \Lambda_\epsilon \mathcal{F}_N^* \mathcal{D}_\epsilon,
\]  

(2.12)

where

\[
\mathcal{F}_N = \frac{1}{\sqrt{N}} \left[ \theta_j^{(i-1)(j-1)} \right]_{i,j=1}^N, \quad \theta_N = \exp \left( \frac{2\pi i}{N} \right), \quad i = \sqrt{-1},
\]  

(2.13)

\[
\mathcal{D}_\epsilon = \text{diag} \left( \epsilon \frac{\pi i}{N} \right)_i, \quad \Lambda_\epsilon = \text{diag} \left( \lambda_k^{(\epsilon)} \right)_i, \quad \lambda_k^{(\epsilon)} = \sum_{j=0}^{N-1} q_j \epsilon^j \theta_N^{-kj}, \quad k = 0, 1, ..., N - 1.
\]  

Here, \( \mathcal{F}_N \) is called a Fourier transform matrix which is unitary. \( \mathcal{F}_N^* (\mathcal{F}_N) \) multiplied with a vector is equivalent to Fourier transform (inverse Fourier transform) of the vector up to a scaling constant. From the definitions of \( \{ \lambda_k^{(\epsilon)} \}_{k=0}^{N-1} \)'s, it is clear that the \( N \) numbers \( \{ \lambda_k^{(\epsilon)} \}_{k=0}^{N-1} \) can be computed within one fast Fourier transform (FFT), which requires only \( O(N \log N) \) flops.

By the fact that \( (D_\epsilon^{-1} \mathcal{F}_N) (\mathcal{F}_N^* D_\epsilon) = I_t \) and (2.12), we know that

\[
\mathcal{R}_\epsilon = \left[ (D_\epsilon^{-1} \mathcal{F}_N) \otimes I_x \right] \left[ (\sqrt{7} I_t + 2 \sqrt{7} \Lambda_\epsilon) \otimes I_x + \tau \sqrt{7} I_t \otimes \mathcal{L}_h \right] \left[ (\mathcal{F}_N^* D_\epsilon) \otimes I_x \right].
\]  

(2.14)

Then, for any given vector \( \mathbf{r} \in \mathbb{R}^{N J} \), the matrix-vector product \( \mathbf{x} = \mathcal{R}_\epsilon^{-1} \mathbf{r} \) can be computed by solving the linear system \( \mathcal{R}_x \mathbf{x} = \mathbf{r} \) in the following PinT pattern

\[
\begin{align*}
\tilde{\mathbf{r}} &= [(\mathcal{F}_N^* D_\epsilon) \otimes I_x] \mathbf{r}, & \text{step-(a)}, \\
[\sqrt{7} + 2 \sqrt{7} \lambda_k^{(\epsilon)}] I_x + \tau \sqrt{7} \mathcal{L}_h) \tilde{x}_k &= \tilde{r}_k, \quad k = 1, 2, ..., N, & \text{step-(b)}, \\
\mathbf{x} &= [(D_\epsilon^{-1} \mathcal{F}_N) \otimes I_x] \tilde{x}, & \text{step-(c)},
\end{align*}
\]  

(2.15)
where \( \tilde{r} = (\tilde{r}_1^T, \tilde{r}_2^T, \ldots, \tilde{r}_N^T)^T, \quad \tilde{x} = (\tilde{x}_1^T, \tilde{x}_2^T, \ldots, \tilde{x}_N^T)^T. \)

By applying FFTs along temporal dimension, we see that the computation of Step-(a) and Step-(c) of (2.15) requires only \( O(JN \log N) \) flops. The most heavy computation burden is to solve the \( N \) many linear systems in Step-(b) of (2.15). But interestingly, these systems are completely independent and therefore the computation is PinT.

From (2.14), we know that \( \mathcal{R}^T \) is also block diagonalizable, i.e.,
\[
\mathcal{R}^T = [(D_x F_N) \otimes I_x]([\sqrt{\tau} I_x + 2 \sqrt{\eta} \Lambda_\tau \otimes I_x + \tau \sqrt{\eta} I_t \otimes \mathcal{L}_h] [[F_N^* D_x^{-1}] \otimes I_x]. \tag{2.16}
\]

Hence, the matrix-vector product \( \mathcal{R}^{-T} \mathcal{r} \) for a given vector \( \mathcal{r} \) can be computed in a PinT manner similar to (2.15).

In summary, the whole process for computing the matrix-vector product \( \mathcal{P}_\epsilon^{-1} \mathcal{w} \) with a given vector \( \mathcal{w} \in \mathbb{R}^{NJ \times 1} \) is PinT, which is why we call \( \mathcal{P}_\epsilon \) as a PinT preconditioner.

3. Spectra of the Preconditioned matrix \( \mathcal{P}_\epsilon^{-1} \mathcal{K} \) and Optimal Convergence of the PCG Solver for the Preconditioned System (2.11). In this section, we are to show that with proper choice of \( \epsilon \), the eigenvalues of the preconditioned matrix are lower and upper bounded by constants in independent of \( N, J \) and \( \gamma \). The uniform boundedness of the spectrum implies an optimal convergence rate of the PCG solver for the preconditioned system.

We estimate the spectrum of \( \mathcal{P}_\epsilon^{-1} \mathcal{K} \) and \( \mathcal{P}_\epsilon^{-1} \mathcal{P} \) first and then combine the estimations together to estimate the spectrum of the preconditioned matrix \( \mathcal{P}_\epsilon^{-1} \mathcal{K} \).

**Proposition 3.1.** \( \mathcal{P} \) is invertible.

**Proof.** Since \( \mathcal{P} = \mathcal{R} \mathcal{R}^T \), it suffices to show the invertibility of \( \mathcal{R} \). From (2.7), we see that \( \mathcal{R} \) is a block triangular matrix whose invertibility is determined by the invertibility of diagonal blocks. Notice that all diagonal blocks of \( \mathcal{R} \) are identical to \( (\sqrt{\tau} + 2 \sqrt{\eta}) I_x + \tau \sqrt{\eta} \mathcal{L}_h \) that is clearly positive definite and thus invertible. Hence, \( \mathcal{R} \) is invertible. The proof is complete. \( \square \)

For any real symmetric matrices \( \mathbf{H}_1, \mathbf{H}_2 \in \mathbb{R}^{m \times m} \), denote \( \mathbf{H}_2 \succ (\text{or } \succeq) \mathbf{H}_1 \) if \( \mathbf{H}_2 - \mathbf{H}_1 \) is real symmetric positive definite (or real symmetric positive semi-definite). Also, \( \mathbf{H}_1 \prec (\text{or } \preceq) \mathbf{H}_2 \) has the same meaning as that of \( \mathbf{H}_2 \succ (\text{or } \succeq) \mathbf{H}_1 \).

Let \( O \) denote zero matrix with proper size.

For any \( O \preceq \mathbf{H} \in \mathbb{R}^{m \times m} \) and \( p \geq 0 \), denote
\[
\mathbf{H}^p := \mathbf{U}^T \text{diag}(d_1^p, d_2^p, \ldots, d_m^p) \mathbf{U},
\]
where \( \mathbf{U}^T \text{diag}(d_1, d_2, \ldots, d_m) \mathbf{U} \) is orthogonal diagonalization of \( \mathbf{H} \). In particular, if \( \mathbf{H} \succ O \), then we write \( (\mathbf{H}^{-1})^p \) as \( \mathbf{H}^{-p} \) for \( p > 0 \).

Denote
\[
\hat{D} = \text{diag}((-1)^k)_{k=1}^N. \tag{3.1}
\]

Let \( e_i \) denote the \( i \)-th column of the \( N \times N \) identity matrix. Denote
\[
1_N = (1; 1; \cdots; 1) \in \mathbb{R}^{N \times 1}.
\]

Then, it is straightforward to verify that
\[
B + B^T = 2 \hat{D} 1_N 1_N^T \hat{D} = 2 \hat{D} 1_N 1_N^T \hat{D}^{-1}, \tag{3.2}
\]
where the last equality is due to \( \hat{D} = \hat{D}^{-1} \).

For a real symmetric matrix \( \mathbf{H} \), let \( \lambda_{\min}(\mathbf{H}) \) and \( \lambda_{\max}(\mathbf{H}) \) denote the minimal and maximal eigenvalues of \( \mathbf{H} \), respectively. For a real square matrix \( \mathbf{C} \), define its symmetric part \( \mathcal{H}(\mathbf{C}) \) as
\[
\mathcal{H}(\mathbf{C}) := \frac{\mathbf{C} + \mathbf{C}^T}{2}.
\]
where $\hat{\text{quotient}}$.

The rest of the proof is devoted to estimating the lower and upper bounds of Rayleigh

circulant matrix is diagonalizable by $F_N$. We state this interesting fact in the following

Proposition 3.3. (see, e.g., [8]) A circulant matrix $C \in \mathbb{C}^{N \times N}$ is diagonalizable

by the $F_N$, i.e.,

$$C = F_N \text{diag}(\sqrt{N} F_N^* C(:, 1)) F_N^*,$$

where $C(:, 1)$ denotes the first column of $C$.

Recall the definition of $R_\sigma$ given in (2.9), we see that

$$\mathcal{H}(R_\sigma) = (\sqrt{\tau} I_t + 2 \sqrt{\eta} \mathcal{H}(B_\sigma)) \otimes I_x + \tau \sqrt{\eta} I_t \otimes \mathcal{L}_h.$$ (3.3)

From the definition of $B_\sigma$ given in (2.10), it is straightforward to verify that

$$\mathcal{H}(B_\sigma) = \hat{D} C_\sigma \hat{D}^{-1} = \hat{D} C_\sigma \hat{D},$$ (3.4)

where $\hat{D}$ is a diagonal matrix defined in (3.1). $C_\sigma$ is a circulant matrix with

$$[1 + \epsilon(-1)^N] 1 - \epsilon(-1)^N e_1 \in \mathbb{R}^{N \times 1},$$

as its first column. Here, $1 \in \mathbb{R}^{N \times 1}$ denotes the vector whose components are all identical to 1 and $e_1 \in \mathbb{R}^{N \times 1}$ denotes the first column of the $N \times N$ identity matrix.

Denote $\hat{F}_N = \hat{D} F_N$. It is clear that $\hat{F}_N$ is a unitary matrix. By Proposition 3.3, $C_\sigma$ is diagonalizable by $F_N$ with the entries of the vector $\sqrt{N} F_N^*[1 + \epsilon(-1)^N] 1 - \epsilon(-1)^N e_1$ as its eigenvalues. By a routine calculation, we obtain the diagonalization formula of $\mathcal{H}(B_\sigma)$ as follows

$$\mathcal{H}(B_\sigma) = \hat{F}_N \Lambda_\sigma \hat{F}_N^*,$$ (3.5)

where $\Lambda_\sigma = N[1 + \epsilon(-1)^N] \text{diag}(e_1) - \epsilon(-1)^N I_t$.

By setting $\epsilon = 0$ in (3.5), we know that $\mathcal{H}(B)$ is also diagonalizable by $\hat{F}_N$ as follows

$$\mathcal{H}(B) = \hat{F}_N \hat{\Lambda} \hat{F}_N^*,$$ (3.6)

Let $\sigma(\cdot)$ denotes the spectrum of a square matrix.

Lemma 3.4. The eigenvalues of $\sigma(P^{-1}K)$ are lower and upper bounded by $\frac{1}{2}$ and 1, respectively, i.e., $\sigma(P^{-1}K) \subset \left[\frac{1}{2}, 1\right]$.

Proof. $P \succ O$ and $K \succ O$ imply that $\sigma(P^{-1}K) = \sigma(P^{-\frac{3}{2}}K P^{-\frac{3}{2}}) \subset (0, +\infty)$ and that eigenvectors of $P^{-1}P$ are all real. Let $(\lambda, x)$ be an eigenpair of $P^{-1}K$. Then,

$$Kx = \lambda Px.$$ (3.7)

Hence,

$$\lambda = \frac{x^T K x}{x^T P x}.$$ (3.7)

The rest of the proof is devoted to estimating the lower and upper bounds of Rayleigh quotient (3.7). From the definitions of $P$ and $K$, we have

$$K = (\sqrt{\tau} I)(\sqrt{\tau} I) + (\sqrt{\eta} G)(\sqrt{\eta} G)^T,$$

$$P = (\sqrt{\tau} I + \sqrt{\eta} G)(\sqrt{\tau} I + \sqrt{\eta} G)^T$$

$$= (\sqrt{\eta} G)(\sqrt{\eta} G)^T + (\sqrt{\tau} I)(\sqrt{\tau} I) + (\sqrt{\tau} I)(\sqrt{\eta} G)^T + (\sqrt{\eta} G)(\sqrt{\tau} I),$$
where \( I = I_t \otimes I_x \) denotes the \((NJ) \times (NJ)\) identity matrix. Denote
\[
c = \sqrt{\eta}G^T x, \quad d = \sqrt{\tau} x.
\]

Then, it is straightforward to verify that
\[
\frac{x^T K x}{x^T P x} = \frac{c^T c + d^T d}{c^T c + d^T d + c^T d + d^T c}
\]
(3.8)

Note that
\[
c^T d + d^T c = \sqrt{\eta}x^T(G + G^T)x = \sqrt{\eta}x^T[4H(B) \otimes I_x + 2\tau I_t \otimes L_h]x.
\]

From (3.6), we know that \( H(B) \succeq O \), which together with \( L_h \succeq O \) implies that \( c^T d + d^T c \geq 0 \). Therefore,
\[
\frac{c^T c + d^T d}{c^T c + d^T d + c^T d + d^T c} \leq 1.
\]
(3.9)

Let \( \langle \cdot, \cdot \rangle \) denote the standard inner product in the Euclidean space. Then, by Cauchy-Schwartz inequality, it follows that
\[
c^T d + d^T c = 2\langle c, d \rangle \leq 2\langle c, c \rangle^{\frac{1}{2}}\langle d, d \rangle^{\frac{1}{2}} \leq \langle c, c \rangle + \langle d, d \rangle = c^T c + d^T d,
\]
and thus \( c^T c + d^T d + c^T d + d^T c \leq 2(c^T c + d^T d) \). That means
\[
\frac{c^T c + d^T d}{c^T c + d^T d + c^T d + d^T c} \geq \frac{c^T c + d^T d}{2(c^T c + d^T d)} = \frac{1}{2},
\]
which together with (3.7), (3.8) and (3.9) implies that
\[
\frac{1}{2} \leq \lambda \leq 1.
\]

The proof is complete. \( \square \)

**Theorem 3.5.** For any \( \epsilon \in (0, 1) \cap \left(0, \frac{\tau}{2\sqrt{\eta}}\right) \), \( P_\epsilon \) is invertible.

**Proof.** Recall that \( P_\epsilon = R_\epsilon R_\epsilon^T \). Hence, to prove the invertibility of \( P_\epsilon \), it suffices to prove the invertibility of \( R_\epsilon \). Let \( (\lambda, x) \) be an eigenpair of \( R_\epsilon \). Then, \( R_\epsilon x = \lambda x \) and thus
\[
x^T R_\epsilon x = \lambda ||x||_2^2 = x^T H(R_\epsilon) x = \Re(\lambda) ||x||_2^2,
\]
where \( \Re(\cdot) \) denotes real part of a complex number. If \( H(R_\epsilon) \succ O \), then
\[
\Re(\lambda) = \frac{x^T H(R_\epsilon) x}{||x||_2^2} > 0,
\]
which implies \( \lambda \neq 0 \). The rest part of this proof is devoted to showing \( H(R_\epsilon) \succ O \).

**Case (i):** \( N \) is an odd number. By (3.5) and \( \epsilon \in (0, 1] \), it is clear that \( H(B_\epsilon) \succeq O \). Combining this with (3.3), we know that \( H(R_\epsilon) \succ O \) in this case.

**Case (ii):** \( N \) is an even number. Denote \( \Lambda_\epsilon = \sqrt{\tau}I_t + 2\sqrt{\eta} \Lambda_\epsilon \). From (3.5) and (3.3), we know that
\[
H(R_\epsilon) \succeq (\sqrt{\tau}I_t + 2\sqrt{\eta} \Lambda_\epsilon(1, 1)) \otimes I_x = (\tilde{F}_N \otimes I_x)(\tilde{\Lambda}_\epsilon \otimes I_x) (\tilde{F}_N^T \otimes I_x).
\]
(3.10)

Hence, to show \( H(R_\epsilon) \succ O \), it suffices to show the diagonal entries of the diagonal matrix \( \tilde{\Lambda}_\epsilon \) are all positive. Since \( \epsilon \in (0, 1] \), \( \tilde{\Lambda}_\epsilon(1, 1) = \sqrt{\tau} + N[1 + \epsilon(-1)^N] - \epsilon(-1)^N = \sqrt{\tau} + N + (N - 1)\epsilon > 0 \). Moreover, since \( \epsilon \in \left(0, \frac{\tau}{2\sqrt{\eta}}\right) \),
\[
\tilde{\Lambda}_\epsilon(i, i) = \sqrt{\tau} - 2\sqrt{\eta}\epsilon > \sqrt{\tau} - 2\sqrt{\eta}\tau/(2\sqrt{\gamma}) = 0.
\]
Hence, $\mathcal{H}(\mathcal{R}_\epsilon) \supset O$.

To summarize the discussion above, we see that $\lambda \neq 0$. By the generality of $\lambda$, we know that $\mathcal{R}_\epsilon$ is invertible and thus $\mathcal{P}_\epsilon$ is invertible. The proof is complete. $\blacksquare$

Let $\rho(\cdot)$ denote the spectral radius of a square matrix.

**Lemma 3.6.**

$$||\tilde{B}\tilde{B}^T||_2 \leq \frac{2T^2}{\tau^2}. $$

**Proof.** A routine calculation yields that

$$(\tilde{B}\tilde{B}^T)(i,j) = \begin{cases} 4(-1)^{j-i}(N-j), & j \geq i, \\ (\tilde{B}\tilde{B}^T)(j,i), & j < i. \end{cases}$$

Because of the equality, it is to check that

$$||\tilde{B}\tilde{B}^T||_1 = ||[\tilde{B}\tilde{B}^T](:,1)||_1 = 4\sum_{i=1}^{N}(N-i) = 2N(N-1) < 2N^2 = \frac{2T^2}{\tau^2},$$

where $[\tilde{B}\tilde{B}^T](:,1)$ denotes the first column of $\tilde{B}\tilde{B}^T$. Then, by symmetry of $\tilde{B}\tilde{B}^T$, we know that

$$||\tilde{B}\tilde{B}^T||_2 = \rho(\tilde{B}\tilde{B}^T) \leq ||\tilde{B}\tilde{B}^T||_1 \leq \frac{2T^2}{\tau^2}. $$

The proof is complete. $\blacksquare$

**Lemma 3.7.** For any $\epsilon \in \left(0, \min\left\{\frac{\tau}{24\sqrt{3}}, \frac{\tau^2}{2\sqrt{6}\gamma T}, \frac{\tau^2}{8\sqrt{3}\gamma T^2}, \frac{1}{3}\right\}\right)$, it holds that $\sigma(\mathcal{P}_\epsilon^{-1}\mathcal{P}) \subset \left[\frac{3}{4}, \frac{1}{2}\right]$.

**Proof.** Since $\epsilon \in \left(0, \frac{1}{4}\right) \cap \left(0, \frac{\sqrt{3}\tau}{24}\right) \subset (0,1] \cap \left(0, \frac{\sqrt{3}\tau}{24}\right)$, Lemma 3.5(i) implies that $\mathcal{P}_\epsilon^{-1}$ exists. Moreover, $\mathcal{P}_\epsilon \supset O$ and $\mathcal{P} \supset O$ imply that $\sigma(\mathcal{P}_\epsilon^{-1}\mathcal{P}) = \sigma(\mathcal{P}_\epsilon^{-1}\mathcal{P}\mathcal{P}_\epsilon^{-1}) \subset (0, +\infty)$ and that eigenvectors of $\mathcal{P}_\epsilon^{-1}\mathcal{P}$ are all real. Let $(\lambda, \mathbf{x})$ be an eigenpair of $\mathcal{P}_\epsilon^{-1}\mathcal{P}$. Then, $\mathcal{P}_\epsilon\mathbf{x} = \lambda\mathcal{P}_\epsilon\mathbf{x}$ and thus

$$\lambda = \frac{\mathbf{x}^T\mathcal{P}_\epsilon\mathbf{x}}{\mathbf{x}^T\mathcal{P}_\epsilon\mathbf{x}}. \quad (3.11)$$

From definition of $\mathcal{P}_\epsilon$ and $\mathcal{P}$, we know that they can be written as

$$\mathcal{P} = [\tau I + 4\sqrt{\gamma} \mathcal{H}(B) + 4\eta \tilde{B}\tilde{B}^T] \otimes I_x + [2\tau \mathbf{\delta}_{\eta} \mathbf{\bar{I}}_t + 4\gamma \mathcal{H}(B)] \otimes \mathcal{L}_h + \tau^2 \eta \mathbf{I}_t \otimes \mathcal{L}_h,$$

$$\mathcal{P}_\epsilon = [\tau I + 4\sqrt{\gamma} \mathcal{H}(B_\epsilon) + 4\eta \tilde{B}\tilde{B}^T] \otimes I_x + [2\tau \mathbf{\delta}_{\eta} \mathbf{\bar{I}}_t + 4\gamma \mathcal{H}(B_\epsilon)] \otimes \mathcal{L}_h + \tau^2 \eta \mathbf{I}_t \otimes \mathcal{L}_h,$$

$$+ 4\eta \epsilon (\tilde{B}\tilde{B}^T + \tilde{B}\tilde{B}^T) \otimes I_x + 4\eta \epsilon^2 (\tilde{B}\tilde{B}^T) \otimes I_x. \quad (3.13)$$

The following inequalities

$$O \preceq \begin{pmatrix} \frac{1}{\sqrt{3}}B + \sqrt{3}\epsilon \tilde{B} \\ \frac{1}{\sqrt{3}}B + \sqrt{3}\epsilon \tilde{B} \end{pmatrix}^T = \epsilon (\tilde{B}\tilde{B}^T + \tilde{B}\tilde{B}^T) + \frac{1}{3} \tilde{B}\tilde{B}^T + 3\epsilon^2 \tilde{B}\tilde{B}^T,$$

$$O \preceq \begin{pmatrix} \frac{1}{\sqrt{3}}B - \sqrt{3}\epsilon \tilde{B} \\ \frac{1}{\sqrt{3}}B - \sqrt{3}\epsilon \tilde{B} \end{pmatrix}^T = -\epsilon (\tilde{B}\tilde{B}^T + \tilde{B}\tilde{B}^T) + \frac{1}{3} \tilde{B}\tilde{B}^T + 3\epsilon^2 \tilde{B}\tilde{B}^T,$$
imply that
\[-\frac{1}{3}BB^T - 3\epsilon^2 \bar{B}\bar{B}^T \preceq \epsilon(B\bar{B}^T + \bar{B}B^T) \preceq \frac{1}{3}BB^T + 3\epsilon^2 \bar{B}\bar{B}^T. \tag{3.14}\]

Moreover, Lemma 3.6 and $0 < \epsilon \leq \frac{\tau^2}{8\sqrt{3}T} \leq \frac{\tau^2}{4\sqrt{\gamma_t}}$ imply that
\[-8\eta^2\bar{B}\bar{B}^T \succeq -\frac{16}\tau I_t \]
\[\geq \left[\frac{-16\eta T^2}{\tau^2} \times \left(\frac{\tau^2}{4\sqrt{6}T}\right)^2\right] I_t = -\frac{\tau}{6} I_t. \tag{3.15}\]

Then,
\[
\tau I_t + 4\sqrt{\gamma}H(B_e) + 4\eta BB^T + 4\eta(B\bar{B}^T + \bar{B}B^T) + 4\eta^2 \bar{B}\bar{B}^T \\
\geq \tau I_t + 4\sqrt{\gamma}H(B_e) + \frac{8}{3}\eta BB^T - 8\eta^2 \bar{B}\bar{B}^T \\
= (\tau - 4\sqrt{(1-N)\epsilon}) I_t + 4\sqrt{(1 + \epsilon(-1)^N}) H(B) + \frac{8}{3}\eta BB^T - 8\eta^2 \bar{B}\bar{B}^T \\
\geq [\tau - 4\sqrt{(1-N)\epsilon - \tau/6}] I_t + 4\sqrt{(1 + \epsilon(-1)^N}) H(B) + \frac{8}{3}\eta BB^T \\
\geq \frac{2}{3} I_t + \frac{8}{3}\sqrt{\gamma}H(B) + \frac{8}{3}\eta BB^T, \tag{3.16}\]
where the first inequality comes from first inequality of (3.14), the first equality comes from (3.5) and (3.6), the second inequality comes from (3.15), the third inequality comes from $\epsilon \in (0, \frac{\tau}{3}] \cap \left(0, \frac{\tau}{24\sqrt{\gamma}}\right]$. By (3.5), (3.6) and $\epsilon \in \left(0, \frac{\tau}{24\sqrt{\gamma}}\right] \cap \left(0, \frac{1}{3}\right]$, we obtain
\[
2\tau^{\frac{7}{3}}\eta^4 I_t + 4\sqrt{\gamma}H(B_e) = [2\tau^{\frac{7}{3}}\eta^4 - 4\tau\epsilon(1-N)] I_t + 4\sqrt{(1 + \epsilon(-1)^N}) H(B) \\
\geq [2\tau^{\frac{7}{3}}\eta^4 - 4\tau \times \frac{\tau}{24\sqrt{\gamma}}] I_t + \frac{8}{3}\gamma H(B) \\
= \frac{11}{6} \tau^{\frac{7}{3}}\eta^4 I_t + \frac{8}{3}\gamma H(B),\]
which together with (3.13), (3.16) and (3.12) implies that
\[
P \geq \frac{2}{3} P.
\]
Applying the above inequality to (3.11), we obtain that
\[
\lambda \leq \frac{3}{2}. \tag{3.17}\]

By Lemma 3.6 and $0 < \epsilon \leq \frac{\tau^2}{8\sqrt{3}T}$, we obtain
\[
16\eta^2\bar{B}\bar{B}^T \preceq \frac{32\eta T^2\epsilon^2}{\tau^2} I_t \\
\preceq \left(\frac{\tau^2}{8\sqrt{3}T}\right)^2 \times \frac{32\eta T^2}{\tau^2} I_t = \frac{\tau}{6} I_t,
\]
which together with (3.14), (3.5), (3.6) and \( \epsilon \in \left(0, \frac{\tau}{24\sqrt{\gamma}}\right] \cap \left(0, \frac{\tau}{24\sqrt{\gamma}}\right)\) implies that
\[
\tau I_t + 4\sqrt{\gamma} \mathcal{H}(B_t) + 4\eta BB^T + 4\eta \epsilon (B B^T + \bar{B} B^T) + 4\eta^2 \bar{B} \bar{B}^T
\leq \tau I_t + 4\sqrt{\gamma} \mathcal{H}(B_t) + \frac{16}{3} \eta BB^T + 16\eta^2 \bar{B} \bar{B}^T
\]
\[
= (\tau - 4\sqrt{\gamma}(-1)N)I_t + 4\sqrt{\gamma}[1 + \epsilon(-1)^N] \mathcal{H}(B) + \frac{16\eta}{3} BB^T + 16\eta^2 \bar{B} \bar{B}^T
\leq [\tau - 4\sqrt{\gamma}(-1)N\epsilon + \tau/6] I_t + 4\sqrt{\gamma}[1 + \epsilon(-1)^N] \mathcal{H}(B) + \frac{16\eta}{3} BB^T
\]
\[
\leq \frac{4\tau}{3} I_t + \frac{16\gamma}{3} \sqrt{\gamma} \mathcal{H}(B) + \frac{16\eta}{3} BB^T. \tag{3.18}
\]

By (3.5), (3.6) and \( \epsilon \in \left(0, \frac{\tau}{24\sqrt{\gamma}}\right] \cap \left(0, \frac{\tau}{24\sqrt{\gamma}}\right] \), we obtain
\[
2\tau \frac{2}{3}\eta \frac{\epsilon}{2} I_t + 4\gamma \mathcal{H}(B_t) = [2\tau \frac{2}{3}\eta \frac{\epsilon}{2} - 4\gamma \epsilon(-1)^N]I_t + 4\gamma[1 + \epsilon(-1)^N] \mathcal{H}(B)
\leq \left[2\tau \frac{2}{3}\eta \frac{\epsilon}{2} + 4\gamma \times \frac{\tau}{24\sqrt{\gamma}}\right] I_t + \frac{16\gamma}{3} \mathcal{H}(B)
\]
\[
= \frac{13}{6} \tau \frac{2}{3}\eta \frac{\epsilon}{2} I_t + \frac{16\gamma}{3} \mathcal{H}(B),
\]

which together with (3.13), (3.18) and (3.12) implies that
\[
\mathcal{P}_{\epsilon} \leq \frac{4}{3} \mathcal{P}.
\]

Applying the above inequality to (3.11), we obtain that
\[
\lambda \geq \frac{3}{4},
\]

which together with (3.17) completes the proof. \( \square \)

With the help of Lemma 3.4 and Lemma 3.7, we obtain an estimation of range of the spectrum of the preconditioned matrix \( \mathcal{P}_{\epsilon}^{-1} \mathcal{K} \) in the following theorem.

**Theorem 3.8.** For any symmetric positive definite matrix \( A \in \mathbb{R}^{n \times n} \), one can define an inner product \( (x, z)_A := x^T A z \), \( x, z \in \mathbb{R}^{n \times 1} \), so that
\[
\sigma(\mathcal{P}_{\epsilon}^{-1} \mathcal{K}) \subset \left[3 \frac{8}{3}, 3 \frac{8}{3}\right].
\]

**Proof.** Since \( \mathcal{P}_{\epsilon}^{-1} \mathcal{K} \) is similar to \( \mathcal{P}_{\epsilon}^{-\frac{1}{2}} \mathcal{K} \mathcal{P}_{\epsilon}^{-\frac{1}{2}} \), we see that \( \mathcal{P}_{\epsilon}^{-1} \mathcal{K} \) has real eigenvalues and real eigenvectors. Let \( (\lambda, x) \) be an eigenpair of \( \mathcal{P}_{\epsilon}^{-1} \mathcal{K} \). Then, \( Kx = \lambda P_{\epsilon} x \) and thus
\[
\lambda = \frac{x^T Kx}{x^T P_{\epsilon} x} = \frac{x^T Kx}{x^T P_{\epsilon} x} \times \frac{x^T P_{\epsilon} x}{x^T P_{\epsilon} x}.
\]

Then, Lemma 3.4 and Lemma 3.7 imply that
\[
\frac{3}{8} \leq \lambda \leq \frac{3}{2},
\]

which completes the proof. \( \square \)

For any symmetric positive definite matrix \( A \in \mathbb{R}^{n \times n} \), one can define an inner product
\[
(x, z)_A := x^T A z, \quad x, z \in \mathbb{R}^{n \times 1},
\]
which induces a vector norm as follows
\[ ||x||_A = (x, x)^{\frac{1}{2}}_A. \]
As \( K \succ O \), one can define inner product as follows
\[ (x, z)_K := x^T K z, \quad x, z \in \mathbb{R}^{NJ \times 1}. \]
Correspondingly, one can define the norm induced by the inner product as follows
\[ ||x||_K := (x, x)^{\frac{1}{2}}_K, \quad x \in \mathbb{R}^{n \times 1}. \]

**Lemma 3.9.** (see [2]) Let \( A_1, A_2 \in \mathbb{R}^{n \times n} \) be symmetric positive definite matrices. Then, the convergence rate of the PCG solver for the preconditioned system \( A_1^{-1} A_2 x = A_1^{-1} b \) can be estimated as follows
\[ ||x^k - x||_{A_2} \leq 2 \left( \frac{\sqrt{c} - \sqrt{\hat{c}}}{\sqrt{c} + \sqrt{\hat{c}}} \right)^k ||x^0 - x||_{A_2}, \]
where \( \hat{c}, \hat{c} \) are any positive numbers satisfying \( \sigma(A_1^{-1} A_2) \subset [\hat{c}, \hat{c}], x^k (k \geq 1) \) denotes the \( k \)th iterative solution by PCG solver, \( x^0 \) denotes an arbitrary initial guess.

Applying Lemma 3.9 to Theorem 3.8, we immediately obtain the convergence result of PCG solver for our preconditioned system (2.11) as stated in the following theorem.

**Theorem 3.10.** Take
\[ \epsilon \in \left( 0, \min \left\{ \frac{\tau^2}{24 \sqrt{\gamma}}, \frac{\tau^2}{2 \sqrt{6 \gamma T}}, \frac{\tau^2}{8 \sqrt{3 \gamma T}}, \frac{1}{3} \right\} \right]. \]
Then, the PCG solver for the preconditioned system (2.11) has a linear convergence rate independent of matrix size \( NJ \), i.e.,
\[ ||v^k - v||_K \leq \frac{2}{3^k} ||v^0 - v||_K, \]
where \( v^k (k \geq 1) \) denotes the \( k \)th iterative solution by PCG solver, \( v^0 \) denotes an arbitrary initial guess.

**Remark 3.1.** Roughly speaking, in Theorem 3.10, the upper bound for \( \epsilon \) is of \( O \left( \frac{\tau^2}{\sqrt{\gamma}} \right) \). That means when \( \epsilon \lesssim \frac{\tau^2}{\sqrt{\gamma}} \), the PCG solver for the preconditioned system (2.11) has a linear convergence rate independent of matrix size and regularization parameter \( \gamma \), which implies that the convergence is optimal.

**4. Numerical Results.** In this section, we test the performance of the proposed PinT preconditioner by several numerical examples. All numerical experiments presented in this section are conducted via MATLAB R2018b on a PC with the configuration: Intel(R) Core(TM) i7-4720HQ CPU 2.60 GHz and 8 GB RAM.

The stopping criterion for PCG solver is set as \( ||r_k||_2 \leq 10^{-8}||r_0||_2 \), where \( r_k = b - K v_k \) denotes the unpreconditioned residual vector at \( k \)th PCG iteration and \( v_0 \) denotes the zero initial guess. The parameter \( \epsilon \) is set as
\[ \epsilon = \frac{1}{2} \min \left\{ \frac{\tau}{24 \sqrt{\gamma}}, \frac{\tau^2}{2 \sqrt{6 \gamma T}}, \frac{\tau^2}{8 \sqrt{3 \gamma T}}, \frac{1}{3} \right\}. \]
It is easy to see that the so evaluated \( \epsilon \) satisfies the assumption presented in Theorem 3.10. Central difference scheme on uniform square grids is adopted to discretize the...
spatial operator $\mathcal{L} = \nabla(a(x) \nabla \cdot)$. When $a(x)$ is a constant function, the linear systems appearing in step-(b) of (2.15) are diagonalizable by fast sine transform and solving each of those linear system requires $O(J \log J)$ flops. For more general diffusion coefficient $a(x)$, we adopt one iteration of V-cycle geometric multigrid method to solve the linear systems in step-(b) of (2.15) and the complexity of the V-cycle iteration is optimal (i.e., proportional to the number of unknowns).

As we mentioned in the introduction part, the authors in [9] also proposed a preconditioner for Schur complement of matrix arising from optimal control problem. Following the idea in [9], we find that the preconditioner proposed in [9] is exactly the matrix $\mathcal{P}$ defined in (2.6). We will compare the performance of $\mathcal{P}$ and our proposed preconditioner $\mathcal{P}_\tau$ in the following experiment. When $\mathcal{P}$ is used as a preconditioner, it requires to invert $\mathcal{P}$ during each PCG-$\mathcal{P}$ iteration. Note that $\mathcal{P} = RR^T$ and $R$ is a block lower triangular matrix. Hence, the inversion of $\mathcal{P}$ resorts to block forward and backward substitutions, which is not PinT.

Recall that the purpose of solving the Schur complement system (2.3) (or equivalently (2.11)) is to compute $[p_{\tau,h}^T, y_{\tau,h}^T]^T$ in (2.1). Let $p_{\tau,h}^*$, $y_{\tau,h}^*$ denote the approximate solution to $p_{\tau,h}$ ($y_{\tau,h}$). Then, we define the error measure as

$$E_{N,J} = \left\| \begin{bmatrix} p_{\tau,h}^* \\ y_{\tau,h}^* \end{bmatrix} - \begin{bmatrix} p_{\tau,h} \\ y_{\tau,h} \end{bmatrix} \right\|_{\infty}.$$

Denote by ‘NoU’, the number of unknowns of the preconditioned Schur complement system (2.11). In other words, ‘NoU’ represents the integer $N \times J$. Denote by ‘Iter’, the iteration number of the PCG solver. Denote by ‘CPU’, the computational time in unit of second. Denote by PCG-$\mathcal{P}$ ($\mathcal{P}$) the PCG solver with preconditioner $\mathcal{P}_\tau$ ($\mathcal{P}$) for the Schur complement system.

**Example 1.** In this example, we consider the minimization problem (1.1) with $a(x_1, x_2) \equiv 1$, $\Omega = (0, 1)^2$, $T = 1$, $f(x_1, x_2, t) = (2\pi^2 - 1) \sin(\pi x_2) \sin(\pi x_1) \exp(-t)$, $g(x_1, x_2, t) = \sin(\pi x_2) \sin(\pi x_1) \exp(-t)$, the analytical solution of which is given by $g(x_1, x_2, t) = \sin(\pi x_1) \sin(\pi x_2) \exp(-t)$, $u \equiv 0$.

The numerical results of PCG-$\mathcal{P}_\tau$ for solving Example 1 are presented in Table 4.1. We observe from Table 4.1 that (i) the iteration numbers of the two solvers in Table 4.1 changes slightly as $N$ or $J$ changes; (ii) the iteration numbers of the two solvers are bounded (increasing first and then decreasing) with respect to the changes of $\gamma$. The boundedness of iteration number of PCG-$\mathcal{P}_\tau$ in Table 4.1 with respect to $N$, $J$ and $\gamma$ supports the theoretical results in Theorem 3.10. Another interesting observation from Table 1 is that the iteration numbers, errors of the two solvers are roughly the same while the CPU cost of PCG-$\mathcal{P}_\tau$ is much smaller than that of PCG-$\mathcal{P}$ especially for large $N$. This is because $\mathcal{P}_\tau$ is a PinT preconditioner while $\mathcal{P}$ is not. The smaller CPU cost of PCG-$\mathcal{P}_\tau$ compared with PCG-$\mathcal{P}$ demonstrates the advantage of a PinT preconditioner.
Table 4.1
Performance of the PCG-\(\mathcal{P}_\epsilon\) and PCG-\(\mathcal{P}\) on Example 1.

| \(\gamma\) | \(N\) | \(J\) | NoU | Iter | CPU(s) | \(E_{N,J}\) | Iter | CPU(s) | \(E_{N,J}\) |
|---|---|---|---|---|---|---|---|---|---|
| \(1e^{-7}\) | 961 | 192200 | 4 | 0.66 | 4.43e-3 | 4 | 4.04 | 4.43e-3 |
| 200 | 3969 | 793800 | 4 | 3.06 | 4.43e-3 | 4 | 12.36 | 4.43e-3 |
| 16129 | 3225800 | 4 | 11.62 | 4.43e-3 | 4 | 42.77 | 4.44e-3 |
| 400 | 961 | 384400 | 4 | 1.36 | 1.99e-3 | 4 | 12.20 | 1.99e-3 |
| 16129 | 6451600 | 4 | 23.38 | 1.99e-3 | 4 | 137.84 | 1.99e-3 |
| \(1e^{-5}\) | 961 | 76880 | 7 | 2.79 | 8.29e-4 | 4 | 1.36 | 1.99e-3 |
| 200 | 3969 | 3175200 | 4 | 11.35 | 8.29e-4 | 4 | 142.26 | 8.29e-4 |
| 16129 | 12903200 | 4 | 46.81 | 8.29e-4 | 4 | 446.34 | 8.29e-4 |
| \(1e^{-3}\) | 961 | 192200 | 6 | 0.90 | 2.45e-3 | 6 | 5.17 | 2.4e-3 |
| 200 | 3969 | 793800 | 6 | 3.77 | 2.45e-3 | 6 | 15.46 | 2.45e-3 |
| 16129 | 3225800 | 6 | 15.70 | 2.45e-3 | 6 | 53.49 | 2.45e-3 |
| \(1e^{-1}\) | 961 | 192200 | 11 | 1.49 | 1.38e-3 | 11 | 9.17 | 1.38e-3 |
| 200 | 3969 | 793800 | 11 | 6.41 | 1.38e-3 | 11 | 26.04 | 1.38e-3 |
| 16129 | 3225800 | 11 | 26.94 | 1.38e-3 | 11 | 95.74 | 1.38e-3 |
| \(1e^{1}\) | 961 | 76880 | 12 | 3.18 | 5.85e-4 | 10 | 23.97 | 5.85e-4 |
| 200 | 3969 | 3175200 | 11 | 13.17 | 7.41e-4 | 11 | 90.67 | 7.41e-4 |
| 16129 | 12903200 | 11 | 325.89 | 7.80e-4 | 11 | 325.89 | 7.80e-4 |
| \(1e^{2}\) | 961 | 192200 | 12 | 3.18 | 5.85e-4 | 10 | 23.97 | 5.85e-4 |
| 200 | 3969 | 793800 | 11 | 6.41 | 1.38e-3 | 11 | 26.04 | 1.38e-3 |
| 16129 | 3225800 | 11 | 26.94 | 1.38e-3 | 11 | 95.74 | 1.38e-3 |
| \(1e^{3}\) | 961 | 76880 | 12 | 3.18 | 5.85e-4 | 10 | 23.97 | 5.85e-4 |
| 200 | 3969 | 3175200 | 11 | 6.41 | 1.38e-3 | 11 | 26.04 | 1.38e-3 |
| 16129 | 12903200 | 11 | 26.94 | 1.38e-3 | 11 | 95.74 | 1.38e-3 |

Note: The table shows the performance of PCG-\(\mathcal{P}_\epsilon\) and PCG-\(\mathcal{P}\) for different values of \(\gamma\), \(N\), and \(J\), with iterations (Iter), CPU time (CPU(s)), and error (\(E_{N,J}\)) for each case.
4.1. The Application of \( \mathcal{P}_r \) to A Locally Controlled Optimal Control Problem. In this subsection, we apply the proposed PinT preconditioner \( \mathcal{P}_r \) to the Schur complement system arising from a locally controlled optimal control problem, and present the related numerical results. The locally controlled optimal control problem is defined as follows

\[
\min_{y,u} \mathcal{L}(y,u) := \frac{1}{2} \|y - g\|_{L^2(\Omega \times (0,T))}^2 + \frac{\gamma}{2} \|u\|_{L^2(\Omega_0 \times (0,T))}^2, \tag{4.1}
\]

subject to a linear wave equation with initial- and boundary-value conditions

\[
\begin{cases}
y_t - Ly = f + \chi_{\Omega_0} u, & \text{in } \Omega \times (0,T), \\
y = 0, & \text{on } \partial \Omega \times (0,T), \\
y(\cdot,0) = y_0, & \Omega.
\end{cases}
\]

The difference between the optimal control problem (1.1) and the locally controlled one (4.1) is that the regularization term \( \frac{\gamma}{2} \|u\|_{L^2(\Omega_0 \times (0,T))}^2 \) is imposed on a subdomain \( \Omega_0 \) with \( \Omega_0 \subset \Omega \) and \( \text{Vol}(\Omega_0) > 0 \). Moreover, the control variable in PDE constraint of (4.1) is weighted by the characteristic function \( \chi_{\Omega_0} \). Here, \( \chi_{\Omega_0} \) denotes the characteristic function of \( \Omega_0 \), which is defined as follows

\[
\chi_{\Omega_0}(x) := \begin{cases} 
1, & x \in \Omega_0, \\
0, & \text{otherwise}.
\end{cases}
\]

Similar to the discussion in Section 1 for (1.1), we can derive a reduced KKT system for (4.1) as follows

\[
\begin{bmatrix}
I & L_2 \\
L_1 & -\gamma^{-1}\chi_{\Omega_0}
\end{bmatrix}
\begin{bmatrix}
y \\
p
\end{bmatrix} =
\begin{bmatrix}
g \\
f
\end{bmatrix}. \tag{4.2}
\]

Applying the same discretization scheme as that used for approximating (1.2), we obtain the following discrete KKT system for (4.2)

\[
\begin{bmatrix}
\frac{\tau}{2}B_2 \otimes I_x \\
B_1 \otimes I_x + \frac{\tau}{2}B_2 \otimes L_h
\end{bmatrix}
\begin{bmatrix}
y_{\tau,h} \\
p_{\tau,h}
\end{bmatrix} =
\begin{bmatrix}
g_{\tau,h} \\
f_{\tau,h}
\end{bmatrix}. \tag{4.3}
\]

Except for \( I_{\Omega_0} \), other notations appearing in (4.3) are already defined in (1.3). Here, \( I_{\Omega_0} \) is a diagonal matrix whose \( i \)th diagonal element is defined as follows

\[
I_{\Omega_0}(i,i) := \begin{cases}
1, & \text{if } i \text{th spatial grid point locates in } \Omega_0, \\
0, & \text{if } i \text{th spatial grid point locates in } \Omega \setminus \Omega_0.
\end{cases}
\]

Applying the same block-diagonal scaling technique used in (1.4) to (4.3), we find that solving the linear system (4.3) reduces to solving the following Schur complement system

\[
(\tau I_1 \otimes I_{\Omega_0} + \eta G G^T)\hat{v} = \hat{b}, \tag{4.4}
\]

for some given vector \( \hat{b} \in \mathbb{R}^{N_J \times 1} \). Clearly, (4.4) is a real symmetric positive definite system, as \( G \) (see the definition in (2.2)) is non-singular. Hence, both PCG-\( \mathcal{P}_r \) and PCG-\( \mathcal{P} \) are applicable to solving (4.4).

Example 2. In this example, we consider the locally controlled optimal control problem (4.1) with

\[
a(x_1,x_2) = 1, \quad \Omega = (0,1)^2, \quad T = 1, \quad f(x_1,x_2,t) = (2\pi^2 - 1) \sin(\pi x_2) \sin(\pi x_1) \exp(-t),
\]

\[
g(x_1,x_2,t) = \sin(\pi x_2) \sin(\pi x_1) \exp(-t), \quad \Omega_0 := (0,1)^2 \setminus (0,0.5)^2.
\]
the analytical solution of which is given by

\[ y(x_1, x_2, t) = \sin(\pi x_1) \sin(\pi x_2) \exp(-t), \quad u \equiv 0. \]

We apply PCG-\( P_\epsilon \) and PCG-\( P \) to solving Example 2, the numerical results of which are presented in Table 2. From Table 2, we see that the CPU cost of PCG-\( P_\epsilon \) is much smaller than that of PCG-\( P \) while the iteration numbers and errors of the two solvers are roughly the same. This again demonstrates the superiority of the proposed PinT preconditioner over the non-PinT preconditioner \( P \) in terms of computational time.

Another observation from Table 4.2 is that the iteration number of the both solvers decreases as \( \gamma \) increases. The reason may be explained as follows. Both \( P_\epsilon \) and \( P \) are originally designed for approximating the matrix \((\tau I_t \otimes I_x + \eta GG^T)\) while in Example 2, \( P_\epsilon \) and \( P \) are used as preconditioners of \((\tau I_t \otimes I_{\Omega_0} + \eta GG^T)\). Recall that \( \eta = \gamma / \tau \). When \( \gamma \) increases, \( \eta GG^T \) becomes dominant and \((\tau I_t \otimes I_{\Omega_0} + \eta GG^T)\) behaves more like \((\tau I_t \otimes I_x + \eta GG^T)\) in spectral sense. Therefore, when \( \gamma \) is not small, \( P_\epsilon \) and \( P \) approximate \((\tau I_t \otimes I_{\Omega_0} + \eta GG^T)\) well in spectral sense and both solvers converges quickly in such case. Hence, \( P_\epsilon \) is an efficient preconditioner for locally controlled optimal control problem when \( \gamma \) is not small.
Table 4.2

Performance of the PCG-$P_1$ and PCG-$P_0$ on Example 2.

| $\gamma$ | $N$   | $J$             | NoU  | PCG-$P_1$          | PCG-$P_0$          |
|----------|-------|-----------------|------|--------------------|--------------------|
|          |       |                 |      | Iter CPU(s) $E_{N,J}$ | Iter CPU(s) $E_{N,J}$ |
|          | 100   | 961             | 96100| 24 1.60 4.61e-3 | 23 8.44 4.61e-3 |
| 1e-4     | 200   | 3969            | 396900| 23 7.15 4.63e-3 | 23 20.32 4.63e-3 |
|          | 16129 | 1612900         | 1612900| 23 29.50 4.63e-3 | 23 64.71 4.63e-3 |
|          | 1e-3  | 200             | 3969 | 25 3.59 2.29e-3 | 23 20.11 2.29e-3 |
|          | 400   | 3969            | 1587600| 25 15.23 1.15e-3 | 23 199.52 1.15e-3 |
|          | 16129 | 6451600         | 1612900| 25 128.73 1.15e-3 | 23 716.28 1.15e-3 |
| 100      | 961   | 96100           | 96100| 24 60.85 2.31e-3 | 23 206.51 2.31e-3 |
| 1e-2     | 200   | 3969            | 793800| 15 2.24 1.25e-3 | 14 12.22 1.24e-3 |
|          | 16129 | 6451600         | 1612900| 15 39.32 1.47e-3 | 14 124.66 1.47e-3 |
| 1e-1     | 200   | 3969            | 793800| 15 9.75 1.42e-3 | 14 36.04 1.42e-3 |
|          | 16129 | 6451600         | 1612900| 15 79.89 7.27e-4 | 14 426.76 7.27e-4 |
| 1        | 200   | 3969            | 1587600| 15 19.87 2.95e-3 | 14 39.27 2.95e-3 |
|          | 16129 | 6451600         | 1612900| 15 15.00 6.68e-4 | 14 30.80 6.68e-4 |
| 1e-1     | 200   | 3969            | 793800| 15 0.77 2.40e-4 | 14 3.75 2.40e-4 |
|          | 16129 | 6451600         | 1612900| 15 3.60 5.59e-4 | 14 9.50 5.59e-4 |
| 1        | 200   | 3969            | 1587600| 15 7.38 2.09e-4 | 14 28.26 2.09e-4 |
|          | 16129 | 6451600         | 1612900| 15 9.99 6.68e-4 | 14 30.80 6.68e-4 |
| 1e-1     | 200   | 3969            | 793800| 15 1.65 3.35e-4 | 14 9.59 3.35e-4 |
|          | 16129 | 6451600         | 1612900| 15 15.00 6.68e-4 | 14 30.80 6.68e-4 |
| 1        | 200   | 3969            | 1587600| 15 3.47 4.54e-4 | 14 28.83 4.54e-4 |
|          | 16129 | 6451600         | 1612900| 15 14.69 5.98e-5 | 14 91.70 5.98e-5 |
| 1e-1     | 200   | 3969            | 793800| 15 2.61 6.56e-4 | 14 22.23 6.56e-4 |
|          | 16129 | 6451600         | 1612900| 15 9.93 1.39e-4 | 14 330.21 1.39e-4 |
5. Concluding Remarks. In this paper, a PinT preconditioner has been proposed for the Schur complement system arising from the parabolic PDE-constrained optimal control problem. Theoretically, we have shown that the spectrum of the preconditioned matrix is lower and upper bounded by positive constants independent of matrix size and the regularization parameter, thanks to which PCG solver for the preconditioned system has been proven to have an optimal convergence rate. Numerical results reported have shown the efficiency of the proposed preconditioning technique and supported the theoretical results.

REFERENCES

[1] D. Abbeloos, M. Diehl, M. Hinze, and S. Vandewalle, Nested multigrid methods for time-periodic, parabolic optimal control problems, Computing and visualization in science, 14 (2011), p. 27.
[2] O. Axelsson and G. Lindskog, On the rate of convergence of the preconditioned conjugate gradient method, Numerische Mathematik, 48 (1986), pp. 499–523.
[3] L. T. Biegler, O. Ghattas, M. Heinkenschloss, D. Keyes, and B. van Bloemen Waanders, Real-time PDE-constrained Optimization, SIAM, 2007.
[4] D. Bini, G. Latouche, and B. Meini, Numerical Methods for Structured Markov Chains, Oxford University Press: New York, 2005.
[5] A. Borzì and V. Schulz, Computational optimization of systems governed by partial differential equations, SIAM, 2011.
[6] M. Kolmbauer and M. Kolmbauer, A preconditioned minres solver for time-periodic parabolic optimal control problems, Numerical Linear Algebra with Applications, 20 (2013), pp. 761–784.
[7] M. Kolmbauer and U. Langer, A robust preconditioned minres solver for distributed time-periodic eddy current optimal control problems, SIAM Journal on Scientific Computing, 34 (2012), pp. B785–B809.
[8] M. K. Ng, Iterative methods for Toeplitz systems, Numerical Mathematics and Scie, 2004.
[9] J. W. Pearson, M. Stoll, and A. J. Wathen, Regularization-robust preconditioners for time-dependent pde-constrained optimization problems, SIAM Journal on Matrix Analysis and Applications, 33 (2012), pp. 1126–1152.
[10] T. Rees, M. Stoll, and A. Wathen, All-at-once preconditioning in PDE-constrained optimization, Kybernetika, 46 (2010), pp. 341–360.
[11] S.-L. Wu and T. Zhou, Diagonalization-based parallel-in-time algorithms for parabolic pde-constrained optimization problems, ESAIM: Control, Optimisation and Calculus of Variations, 26 (2020), p. 88.