A sine transform based preconditioned MINRES method for all-at-once systems from evolutionary partial differential equations

Sean Hon\textsuperscript{1}\textsuperscript{*} and Stefano Serra-Capizzano\textsuperscript{2,3}

\textsuperscript{1}Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong
\textsuperscript{2}Department of Science and High Technology, University of Insubria, Como, Italy
\textsuperscript{3}Department of Information Technology, Uppsala University, Uppsala, Sweden

*Corresponding author. Email: seanyshon@hkbu.edu.hk

Abstract

In this work, we propose a simple yet generic preconditioned Krylov subspace method for a large class of nonsymmetric block Toeplitz all-at-once systems arising from discretizing evolutionary partial differential equations. Namely, our main result is a novel symmetric positive definite preconditioner, which can be efficiently diagonalized by the discrete sine transform matrix. More specifically, our approach is to first permute the original linear system to obtain a symmetric one, and subsequently develop a desired preconditioner based on the spectral symbol of the modified matrix. Then, we show that the eigenvalues of the preconditioned matrix sequences are clustered around ±1, which entails rapid convergence, when the minimal residual method is devised. Alternatively, when the conjugate gradient method on normal equations is used, we show that our preconditioner is effective in the sense that the eigenvalues of the preconditioned matrix sequence are clustered around the unity. An extension of our proposed preconditioned method is given for high-order backward difference time discretization schemes, which applies on a wide range of time-dependent equations. Numerical examples are given to demonstrate the effectiveness of our proposed preconditioner, which consistently outperforms an existing block circulant preconditioner discussed in the relevant literature.

Keywords: sine transform based preconditioners; parallel-in-time; Krylov subspace methods; MINRES; all-at-once discretization; block Toeplitz systems

MSC: 15B05; 65F08; 65F10; 65M22

1 Introduction

Over the past few years, there has been a growing interest on developing effective preconditioners for solving the all-at-once linear systems stemming from evolution-
ary partial differential equations (PDEs); see for instance [32, 31, 23, 22, 19, 27, 28, 30, 42] and references therein. Instead of solving PDEs in a sequential manner, this class of parallel-in-time (PinT) methods solves all unknowns simultaneously by constructing a large linear system which is composed of smaller linear systems at each time levels. Our proposed method in this work belongs to the diagonalization-based all-at-once methods [17], along with [32, 27]. Related PinT methods include space-time multigrid [18, 26], multigrid reduction in time [14, 12], and parareal method [29, 19]. For a survey on the development of these PinT methods, we refer the readers to [16] and the references therein.

As a model problem, we consider the following initial-boundary problem for the heat equation

\[
\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= \nabla (a(x)\nabla u(x,t)) + f(x,t), \quad (x,t) \in \Omega \times (0,T], \\
u &= g, \\
u(x,0) &= u_0(x), \\
\end{aligned}
\]

\[x \in \Omega.\]

where \(\Omega\) is open, \(\partial \Omega\) denotes boundary of \(\Omega\), and \(a, f, g, u_0\) are all given functions.

After discretizing the spatial domain with a mesh and using the simple two-level \(\theta\)-method for time discretization with \(n\) time-steps of size \(\tau = \frac{T}{n}\), we get

\[
M_m \left( \frac{u_m^{(k+1)} - u_m^{(k)}}{\tau} \right) = -K_m (\theta u_m^{(k+1)} + (1-\theta)u_m^{(k)}) + \theta f_m^{(k+1)} + (1-\theta)f_m^{(k)},
\]

where \(M_m, K_m \in \mathbb{R}^{m \times m}\) are the mass matrix and the stiffness matrix approximating \(-\nabla (a(\nabla \cdot)\nabla)\), respectively, in the standard finite element terminology, \(u_m^{(k)} = [u_1^{(k)}, \ldots, u_m^{(k)}]^T\), \(f_m^{(k)} = [f_1^{(k)}, \ldots, f_m^{(k)}]^T\), and \(\theta \in [0,1]\). The forward Euler method corresponds to the choice \(\theta = 0\), the backward Euler method to \(\theta = 1\), while the Crank-Nicolson method is associated with \(\theta = 1/2\).

The discrete equations to be solved are described below

\[(M_m + \theta \tau K_m)u_m^{(k+1)} = (M_m - (1-\theta)\tau K_m)u_m^{(k)} + \theta \tau f_m^{(k+1)} + (1-\theta)\tau f_m^{(k)}.
\]

Instead of solving the above equations for \(u_m^{(k)}\) sequentially, for \(k = 1, 2, \ldots, n\), we solve the following equivalent all-at-once system

\[
\begin{bmatrix}
u_m^{(1)} \\
u_m^{(2)} \\
u_m^{(3)} \\
\vdots \\
u_m^{(n)} \\
\end{bmatrix} = \begin{bmatrix}
\theta \tau f_m^{(1)} + (1-\theta)\tau f_m^{(0)} + (M_m - (1-\theta)\tau K_m)u_m^{(0)} \\
\theta \tau f_m^{(2)} + (1-\theta)\tau f_m^{(1)} \\
\theta \tau f_m^{(3)} + (1-\theta)\tau f_m^{(2)} \\
\vdots \\
\theta \tau f_m^{(n)} + (1-\theta)\tau f_m^{(n-1)} \\
\end{bmatrix}
\]

where

\[
T_H = \begin{bmatrix}
M_m + \theta \tau K_m \\
-M_m + (1-\theta)\tau K_m \\
\vdots \\
-M_m + (1-\theta)\tau K_m \\
-M_m + (1-\theta)\tau K_m \\
M_m + \theta \tau K_m \\
\end{bmatrix}
\]

(2)
is a \( mn \) by \( mn \) nonsymmetric block Toeplitz matrix, which is generated by the matrix-valued function

\[
g_\theta(x) = M_m + \theta \tau K_m + \left( -M_m + (1 - \theta) \tau K_m \right) e^{ix}.
\]

According to the notion of generating function reported in Section 2 (see also [20, 21] and the references there reported), it is noted that if \( K_m \) and \( M_m \) commute then \( A(0) \) and \( A(1) \) commute. If one uses a finite element formulation to discretize in space for (1), then \( M_m \) and \( K_n \) are simultaneously diagonalizable, provided that a uniform grid is used. Alternatively, if finite difference methods are used for (1), then \( M_m \), being exactly the identity matrix \( I_m \) in this case, always commutes with \( K_m \) (see [32, Section 3.1.1] for a discussion).

Therefore, throughout this work, the following assumptions on both \( M_m \) and \( K_m \) are made, which are compatible with [27, Section 2]:

1. Both \( M_m \) and \( K_m \) are real symmetric positive definite (SPD);
2. Both \( M_m \) and \( K_m \) are sparse, i.e., they have only \( O(m) \) nonzero entries.
3. Both \( M_m \) and \( K_m \) commute.

Instead of directly solving (2), we consider the permuted linear system \( \mathcal{Y}T_H u = \mathcal{Y}f_H \), where

\[
\mathcal{Y}T_H = \begin{bmatrix}
A(1) & A(0) \\
A(0) & A(1) \\
A(1) & A(0) \\
A(0) & A(1)
\end{bmatrix}.
\]

Note that \( \mathcal{Y} = Y_n \otimes I_m \) with \( Y_n \in \mathbb{R}^{n \times n} \) being the anti-identity matrix or the flip matrix that is \( [Y_n]_{j,k} = 1 \) if and only if \( j + k = n + 1 \) and \( [Y_n]_{j,k} = 0 \) otherwise. Clearly, \( \mathcal{Y}T_H \) is symmetric since \( L_m \) is assumed symmetric. Thus, we can then deploy a symmetric Krylov subspace method such as the minimal residual (MINRES) method and design an effective preconditioner for \( \mathcal{Y}T_H \), whose convergence depends only on the eigenvalues.

While a simple block circulant preconditioner was proposed for \( \mathcal{Y}T_H \) in [32], its performance for the ill-conditioned systems is in fact unsatisfactory as discussed in [25]. Motivated by overcoming such a limitation of block circulant preconditioners, we propose the following SPD preconditioner for \( \mathcal{Y}T_H \), that can be diagonalized by the discrete sine transform matrix

\[
\mathcal{P}_H = \begin{bmatrix}
A^2(0) + A^2(1) & A(0)A(1) \\
A(0)A(1) & A^2(0) + A^2(1) \\
& \ddots & \ddots \\
& & \ddots & A(0)A(1) \\
& & & A^2(0) + A^2(1)
\end{bmatrix},
\]

which is constructed based on approximating the asymptotic eigenvalue distribution of \( \mathcal{Y}T_H \). We remind that in a pure Toeplitz setting the algebra of matrices diagonalized by the (real) orthogonal sine transform (i.e. the so-called \( \tau \) algebra [4]) was extensively used in the 90s (see [10, 11, 35, 37] and references therein), while quite recently the approach based on \( \tau \) preconditioning gained further attention in the
context of approximated fractional differential equations (see [1, 13] and references therein). Here in this work we propose its use in a different setting.

In particular, we will show that the eigenvalues of the preconditioned matrix sequence \( \{P_n^{-1}YH \}_n \) are clustered around \( \pm 1 \), which ensures fast convergence when MINRES is employed. In general, as mentioned in [11, Chapter 6], the convergence study of preconditioning strategies for nonsymmetric problems is heuristic, since descriptive convergence bounds are usually not available for the generalized minimal residual (GMRES) method or any of the other applicable nonsymmetric Krylov subspace iterative methods.

The paper is organized as follows. In Section 2, we review some preliminary results on block Toeplitz matrices and matrix-valued functions. We present our main results in Section 3 where our proposed preconditioner and its effectiveness are provided. An extension of our preconditioning method is given in Section 4. Numerical tests are given in Section 5 to support the our proposed preconditioners.

2 Preliminaries

In the following subsections, we provide some useful background knowledge about block Toeplitz matrices and matrix functions.

2.1 Block Toeplitz matrices

We let \( L^1([\pi, \pi], \mathbb{C}^{m \times m}) \) be the Banach space of all matrix-valued functions that are Lebesgue integrable over \([-\pi, \pi]\). The \( L^1 \)-norm induced by the trace norm over \( \mathbb{C}^{m \times m} \) is

\[
\|f\|_{L^1} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \|f(x)\|_{tr} \, dx < \infty,
\]

where \( \|A_n\|_{tr} := \sum_{j=1}^{n} \sigma_j(A_n) \) denotes the trace norm of \( A_n \in \mathbb{C}^{n \times n} \). The block Toeplitz matrix generated by \( f \in L^1([\pi, \pi], \mathbb{C}^{m \times m}) \) is denoted by \( T_{(n,m)}[f] \), namely

\[
T_{(n,m)}[f] = \begin{bmatrix}
A_{(0)} & A_{(-1)} & \cdots & A_{(-n+1)} \\
A_{(1)} & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & A_{(-1)} \\
A_{(n-1)} & \cdots & A_{(1)} & A_{(0)}
\end{bmatrix} \in \mathbb{C}^{mn \times mn},
\]

where the Fourier coefficients of \( f \) are

\[
A_{(k)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)e^{-ikx} \, dx \in \mathbb{C}^{m \times m}, \quad k = 0, \pm 1, \pm 2, \ldots.
\]

The function \( f \) is called the generating function/symbol of \( T_{(n,m)}[f] \). For thorough discussions on the related properties of (multilevel) block Toeplitz matrices, we refer the readers to [33, 24, 21] and references therein.

Before discussing the asymptotic singular value/spectral distribution of \( T_{(n,m)}[f] \) associated with \( f \), which is crucial to develop our preconditioning theory, we introduce the following definition.

Let \( C_c(\mathbb{C}) \) (or \( C_c(\mathbb{R}) \)) be the space of complex-valued continuous functions defined on \( \mathbb{C} \) (or \( \mathbb{R} \)) with bounded support.

**Definition 2.1.** [24] Let \( \{A_{(n,m)}\}_n \) be a sequence of \( mn \)-by-\( mn \) matrix.
1. We say that \([A_{(n,m)}]_n\) has an asymptotic singular value distribution described by an \(m\times m\) matrix-valued \(f\) if

\[
\lim_{n \to \infty} \frac{1}{mn} \sum_{j=1}^{mn} F(\sigma_j(A_{(n,m)})) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{m} \sum_{j=1}^{m} F(\sigma_j(f(x))) \, dx, \quad \forall F \in C_c(\mathbb{R})
\]

and we write \([A_{(n,m)}]_n \sim_\sigma f\).

2. We say that \([A_{(n,m)}]_n\) has an asymptotic spectral distribution described by an \(m\times m\) matrix-valued \(f\) if

\[
\lim_{n \to \infty} \frac{1}{mn} \sum_{j=1}^{mn} F(\lambda_j(A_{(n,m)})) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{m} \sum_{j=1}^{m} F(\lambda_j(f(x))) \, dx, \quad \forall F \in C_c(\mathbb{C})
\]

and we write \([A_{(n,m)}]_n \sim_\lambda f\).

Before presenting our main preconditioning results, we introduce the following notation. Given \(D \subset \mathbb{R}^k\) with \(0 < \mu_k(D) < \infty\), we define \(\bar{D}\) as \(D \cup D_p\), where \(p \in \mathbb{R}^k\) and \(D_p = p + D\), with the constraint that \(D\) and \(D_p\) have non-intersecting interior part, i.e. \(D^o \cap D_p^o = \emptyset\). In this way, we have \(\mu_k(\bar{D}) = 2\mu_k(D)\). Given any \(g\) defined over \(D\), we define \(\psi_g\) over \(\bar{D}\) in the following fashion

\[
\psi_g(x) = \begin{cases} 
  g(x), & x \in D, \\
  -g(x-p), & x \in D_p, \quad x \notin D.
\end{cases}
\]

(7)

**Theorem 2.1.** \([14, \text{Theorem 3.4}]\) Suppose \(f \in L^1([-\pi, \pi], \mathbb{C}^{m \times m})\) has Hermitian Fourier coefficients. Let \(T_{(n,m)}[f] \in \mathbb{C}^{mn \times mn}\) be the block Toeplitz matrix generated by \(f\) and let \(Y_{(n,m)} = Y_n \otimes I_m \in \mathbb{R}^{mn \times mn}\). Then

\[
\{Y_{(n,m)}T_{(n,m)}[f]\}_n \sim_\lambda \psi_{\|f\|}, \quad ||f|| = (ff^*)^{1/2},
\]

over the domain \(\bar{D}\) with \(D = [0, 2\pi]\) and \(p = -2\pi\), where \(\psi_{\|f\|}\) is defined in (7). That is

\[
\lim_{n \to \infty} \frac{1}{mn} \sum_{j=1}^{mn} F(\lambda_j(Y_{(n,m)}T_{(n,m)}[f]))) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{m} \sum_{j=1}^{m} F(\lambda_j(||f||x(x))) \, dx,
\]

where \(\lambda_j(||f||x(x)), j = 1, 2, \ldots, m,\) are the eigenvalue functions of \(\|f\|\).

As for the symmetrized matrix \(\mathcal{Y}T_H\) given in (4), we can see by \([15, 24]\) that their eigenvalues are distributed as \(\pm ||g_0||\). By Theorem 2.1, \(\mathcal{Y}T_H\) is always symmetric indefinite when \(n\) is sufficiently large, which justifies the use of MINRES in this work.

### 2.2 Matrix functions

In this subsection, several useful results on functions of matrices are presented.

If \(F\) is analytic on a simply connected open region of the complex plane containing the interval \([-1, 1]\), there exist ellipses with foci in \(-1\) and \(1\) such that \(F\) is analytic in their interiors. Let \(\alpha > 1\) and \(\beta > 0\) be the half axes of such an ellipse with \(\sqrt{\alpha^2 - \beta^2} = 1\). Such an ellipse, denoted by \(E_\mathcal{X}\), is completely specified once the number \(\mathcal{X} := \alpha + \beta\) is known.
Theorem 2.2 (Bernstein’s theorem). [3, Theorem 2.1] Let the function $F$ be analytic in the interior of the ellipse $E_X$ with $X > 1$ and continuous on $E_X$. In addition, suppose $F(x)$ is real for real $x$. Then, the best approximation error

$$E_k(F) := \inf \{ \| F - p \|_{\infty} : \deg(p) \leq k \} \leq \frac{2M(X)}{X^k(X - 1)},$$

where $\deg(p)$ denotes the degree of the polynomial $p(x)$ and

$$\| F - p \|_{\infty} = \max_{-1 \leq x \leq 1} | F(x) - p(x) |, \quad M(X) = \max_{x \in E_X} \{| F(x) | \}.$$ 

Let $A_n$ be an $n \times n$ symmetric matrix and let $[\lambda_{\text{min}}, \lambda_{\text{max}}]$ be the smallest interval containing $\sigma(A_n)$. If we introduce the linear affine function

$$\psi(\lambda) = \frac{2\lambda - (\lambda_{\text{min}} + \lambda_{\text{max}})}{\lambda_{\text{max}} - \lambda_{\text{min}}},$$

then $\psi([\lambda_{\text{min}}, \lambda_{\text{max}}]) = [-1, 1]$ and therefore the spectrum of the symmetric matrix

$$B_n := \psi(A_n) = \frac{2}{\lambda_{\text{max}} - \lambda_{\text{min}}} A_n - \frac{\lambda_{\text{min}} + \lambda_{\text{max}}}{\lambda_{\text{max}} - \lambda_{\text{min}}} I_n$$

is contained in $[-1, 1]$. Given a function $f$ analytic on a simply connected region containing $[\lambda_{\text{min}}, \lambda_{\text{max}}]$ and such that $f(\lambda)$ is real when $\lambda$ is real, the function $F = f \circ \psi^{-1}$ satisfies the assumptions of Bernstein’s theorem.

In the special case where $A_n$ is SPD and $f(x) = x^{-1/2}$ that are of our interest in this work, we apply Bernstein’s result to the function

$$F(x) = \frac{1}{\sqrt{(b-a)x + a+b}}, \quad (8)$$

where $a = \lambda_{\text{min}}(A_n)$, $b = \lambda_{\text{max}}(A_n)$, and $1 < X < \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1}$ with the spectral condition number of $A_n$ being $\kappa = b/a$.

3 Main results

In this section, we provide our results on the proposed preconditioner $P$ defined by [3], whose design is based on the following spectral symbol

$$|g_\theta|^2 = A_{0}^{2} + A_{1}^{2} + A_{0} A_{1} e^{-i\theta} + A_{0} A_{1} e^{i\theta} = A_{0}^{2} + A_{1}^{2} + 2 A_{0} A_{1} \cos(\theta). \quad (9)$$

Due to the fact that $P = \sqrt{T_{(n,m)}[|g_\theta|^2]}$, it can be regarded as an optimal preconditioner for $\mathcal{Y}T$, in the sense of the spectral distribution theory developed in our work [15]. We discuss mainly MINRES combined with our proposed preconditioner, and related issues such as implementations and convergence analysis are given as well.

3.1 Preconditioning for heat equations

In this section, we provide a MINRES approach for $\mathcal{Y}T_H u = \mathcal{Y}f_H$. 

6
3.1.1 Implementations

We first discuss the fast computation of $\mathcal{Y}T_H v$ for any given vector $v$. Since both $M_m$ and $K_m$ are sparse matrices, $T_H$ is sparse. Hence, computing the matrix-vector product $T_H v$ only requires linear complexity of $O(mn)$. Finally, computing $\mathcal{Y}T_H v$ needs the same complexity since $\mathcal{Y}$ simply imposes a reordering on the vector $T_H v$.

Alternatively, due to the fact that $T_H$ itself is a block Toeplitz matrix, it is well-known that the product $\mathcal{Y}T_H v$ can be computed in $O(mn \log n)$ operations using FFTs and the related storage is of $O(mn)$, where $m$ can be regarded as a fixed constant and $n$ is the effective dimensional parameter.

We first indicate that $P$ has the following decomposition

$$P_H = \sqrt{T_{n,m}}[|y_0|^2] = \sqrt{I_n \otimes (A^2_0 + A^2_1) + P_n \otimes 2(A_0 A_1)}$$

where

$$P_n = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & \cdots & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & \frac{1}{2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \frac{1}{2} & \cdots & \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

is a tridiagonal Toeplitz matrix which has the eigendecomposition $P_n = S_n D_n S_n$ with $S_n = \sqrt{\frac{2}{\pi+1}} \left[ \sin \left( \frac{i j \pi}{n+1} \right) \right]_{i,j=1}^{n} \in \mathbb{R}^{n \times n}$ being the symmetric discrete sine transform matrix. Hence,

$$P_H = \sqrt{I_n \otimes U_m (A^2_0 + A^2_1) U^T_m + P_n \otimes (U_m 2A_0 A_1 U^T_m)}$$

$$= \sqrt{(S_n \otimes U_m) \left( I_n \otimes (A^2_0 + A^2_1) + D_n \otimes 2A_0 A_1 \right) (S_n \otimes U_m)^T}$$

$$= (S_n \otimes U_m) \sqrt{I_n \otimes (A^2_0 + A^2_1) + D_n \otimes 2A_0 A_1} (S_n \otimes U_m)^T.$$

The product $z = P_H^{-1} v$ can be computed via the following three step procedures:

1. Compute $\tilde{v} = (S_n \otimes U^T_m)v$;
2. Compute $\tilde{z} = \left( \sqrt{I_n \otimes (A^2_0 + A^2_1) + D_n \otimes 2A_0 A_1} \right) \tilde{v}$;
3. Compute $z = (S_n \otimes U^T_m)\tilde{z}$.

When both $M_m$ and $K_m$ are diagonalizable by $U_m = S_m$, which holds true when the spatial discretization is a finite difference/element method with a uniform square grid and a constant diffusion coefficient function $a(x)$, the matrix-vector product $z = P_H^{-1} v$ can be computed efficiently in $O(n m (\log m + \log n))$ operations using fast sine transforms with a storage is of order $O(nm)$.
### 3.1.2 Eigenvalue analysis of $\mathcal{P}_H^{-1}\mathcal{Y}_H$

Before showing the eigenvalues of $\mathcal{P}_H^{-1}\mathcal{Y}_H$ are clustered, we first introduce the following block circulant matrix as an auxiliary

$$
\mathcal{C}_H = \begin{bmatrix}
A_{(0)}^2 + A_{(1)}^2 & A_{(0)}A_{(1)} & A_{(0)}A_{(1)} \\
A_{(0)}A_{(1)} & A_{(0)}^2 + A_{(1)}^2 & \ddots \\
& \ddots & \ddots & A_{(0)}A_{(1)} \\
& & \ddots & A_{(0)}^2 + A_{(1)}^2
\end{bmatrix}.
$$

By further introducing the following Strang type [40] block circulant preconditioner which was proposed in [32] for $\mathcal{Y}_H$

$$
\mathcal{S}_H = \begin{bmatrix}
A_{(0)} & A_{(1)} \\
A_{(1)} & \ddots & \ddots \\
& \ddots & \ddots & A_{(1)} \\
& & \ddots & A_{(0)}
\end{bmatrix},
$$

we indicate that $\mathcal{C}_H$ can be rewritten as

$$
\mathcal{C}_H = \sqrt{\mathcal{S}_H^T\mathcal{S}_H} = \sqrt{\mathcal{S}_H\mathcal{S}_H^T}.
$$

**Remark 3.1.** In addition to $\mathcal{C}_H$, one can also define an optimal type [8] block circulant preconditioner for $\mathcal{Y}_H$, which was recently proposed in [23] for $\mathcal{Y}_H$. Since both the Strang and the optimal preconditioners are known to have similar convergence behaviours (see [7] for an exhaustive overview in this regard), we in this work only focus on $\mathcal{C}_H$.

The following proposition guarantees the effectiveness of $\mathcal{C}_H$ as a preconditioner for $\mathcal{Y}_H$, showing that the eigenvalues of $\mathcal{C}_H^{-1}\mathcal{Y}_H$ are clustered around ±1 which ensures fast convergence of MINRES. However, as discussed in [25] and shown in the numerical examples to be given in Section 5, $\mathcal{C}_H$ does not work well in the ill-conditioned cases in general.

**Proposition 3.1.** [32, Theorem 4] Let $\mathcal{Y}_H, \mathcal{C}_H \in \mathbb{R}^{mn \times mn}$ be defined in [4] and [11], respectively. Then,

$$
\mathcal{C}_H^{-1}\mathcal{Y}_H = \mathcal{Q}_0 + \mathcal{R}_0,
$$

where $\mathcal{Q}_0$ is symmetric and orthogonal, and rank($\mathcal{R}_0$) ≤ $m$.

Now, we turn our focus on the following lemma and proposition, which will be helpful to showing our main result.

**Lemma 3.2.** Let $\mathcal{C}_H, \mathcal{P}_H \in \mathbb{R}^{mn \times mn}$ be defined in [11] and [5], respectively. Then,

$$
\text{rank}(\mathcal{C}_H^{2K} - \mathcal{P}_H^{2K}) \leq 2Km,
$$

for some positive integer $K$ provided that $n > 2Km$. 

8
Proof. Exploiting the simple structures of both $C^2_H$ and $P^2_H$, we have by direct computations

\[
C_H^{2n_\alpha} (C^2_H - P^2_H) P_H^{2n_\beta} = \begin{bmatrix} * & \cdots & * & \cdots & * \\ \vdots & \ddots & \vdots & & \vdots \\ * & \cdots & * & \cdots & * \\ \vdots & \ddots & \vdots & & \vdots \\ * & \cdots & * & \cdots & * \end{bmatrix}
\]

for integer values $n_\alpha$ and $n_\beta$, where * represents a nonzero entry. Namely, $C_H^{2n_\alpha} (C^2_H - P^2_H) P_H^{2n_\beta}$ is a block matrix with four blocks in its four corners, and each block is of size $(n_\alpha + 1)m \times (n_\beta + 1)m$. Thus,

\[
C_H^{2K} - P_H^{2K} = \sum_{i=0}^{K-1} (C_H^{2K-2i} P_H^{2i} - C_H^{2K-2i} P_H^{2i+2})
\]

\[
= \sum_{i=0}^{K-1} C_H^{2K-2i} (C^2_H - P^2_H) P_H^{2i}
\]

is also a block matrix with four blocks in its four corners and each of them is of size $Km \times Km$, provided that $n > 2Km$. Hence, we have $\text{rank}(C_H^{2K} - P_H^{2K}) \leq 2Km$. □

Remark 3.2. The computational lemma used in the proof of Lemma 3.1 was first given in [34] Lemma 3.11.

Proposition 3.3. Let $C_H, P_H \in \mathbb{R}^{mn \times mn}$ be defined in (11) and (5), respectively. Then for any $\epsilon > 0$ there exists an integer $K$ such that for all $n > 2Km$

\[
C_H^{-1} - P_H^{-1} = \mathcal{E} + \mathcal{R}_1,
\]

where $\|\mathcal{E}\|_2 \leq \epsilon$ and $\text{rank}(\mathcal{R}_1) \leq 2Km$.

Proof. Let $f(x) = x^{-1/2}$ and $F(x)$ be defined in equation (8). By Theorem 2.2 there exists a polynomial $p_K$ with degree less than or equal to $K$ such that

\[
\|C_H^{-1} - p_K(C_H^2)\|_2 = \|(C_H^2)^{-1/2} - p_K(C_H^2)\|_2 = \max_{x \in \sigma(C_H^2)} |F(x) - p_K(x)|
\]

\[
\leq \|F - p_K(x)\|_\infty 
\leq 2M(\chi_{C_H^2}) \frac{1}{\chi_{C_H^2}}.
\]

\[
\|P_H^{-1} - p_K(P_H^2)\|_2 = \|(P_H^2)^{-1/2} - p_K(P_H^2)\|_2 = \max_{x \in \sigma(P_H^2)} |F(x) - p_K(x)|
\]

\[
\leq \|F - p_K(x)\|_\infty 
\leq 2M(\chi_{P_H^2}) \frac{1}{\chi_{P_H^2}}.
\]

where

\[
1 < \chi_{C_H^2} < \frac{\sqrt{\chi_{C_H^2}} + 1}{\sqrt{\chi_{C_H^2}} - 1}, \quad 1 < \chi_{P_H^2} < \frac{\sqrt{\chi_{P_H^2}} + 1}{\sqrt{\chi_{P_H^2}} - 1}.
\]
κ_{C^2_H} and κ_{P^2_H} are the condition numbers of C^2_H and P^2_H, respectively. Thus, for any ε > 0 there exists an integer K such that
\[ \|C^{-1}_H - p_K(C^2_H)\|_2 \leq \epsilon \quad \text{and} \quad \|P^{-1}_H - p_K(P^2_H)\|_2 \leq \epsilon. \]

Also, we have
\[ p_K(C^2_H) - p_K(P^2_H) = \sum_{i=0}^{K} a_i (C^2_i - P^2_i), \]
where \[ R_1 := R.H. \]

By Lemma 3.2, we know that \( R_1 \) has the same sparsity structure as that of \( C^2_K - P^2_K \). Consequently, we deduce \( \text{rank}(R_1) \leq 2Km \).

We then obtain
\[ C^{-1}_H - P^{-1}_H = C^{-1}_H - p_K(C^2_H) + p_K(P^2_H) - P^{-1}_H + p_K(C^2_H) - p_K(P^2_H), \]
where \( \|E\|_2 \leq 2\epsilon \) and \( \text{rank}(R_1) \leq 2Km \). Therefore, the proof is concluded.

**Theorem 3.4.** Let \( YT_H, P_H \in \mathbb{R}^{mn \times mn} \) be defined in (4) and (5), respectively. Then for any \( \epsilon > 0 \) there exists an integer \( K \) such that for all \( n > 2Km \)
\[ P^{-1}_H YT_H = Q_H + \epsilon H + R_H, \]
where \( Q_H \) is both symmetric and orthogonal, \( \|\epsilon_H\|_2 \leq \epsilon \), and \( \text{rank}(R_H) \leq (2K + 1)m \).

**Proof.** By Proposition 3.1, we can write
\[ C^{-1}_H YT_H = Q_0 + R_0, \]
where \( \text{rank}(R_0) \leq m \).

By Proposition 3.3, we then have
\[ P^{-1}_H YT_H = (C^{-1}_H - \epsilon - R_1)YT_H = Q_0 + R_0 - \epsilon YT_H - R_1 YT_H = Q_0 - \epsilon YT_H + R_0 - R_1 YT_H, \]
where \( \text{rank}(R_H) \leq \text{rank}(R_0) + \text{rank}(R_1 YT_H) \leq (2K + 1)m \)
and
\[ \|\epsilon_H\|_2 = \|\epsilon YT_H\|_2 \leq \|YT_H\|_2 \epsilon. \]

Note that
\[ \|YT_H\|_2 = \|T\|_2 \leq \|g_0\|_{\infty}. \]

by using the general inequalities in [6, Corollary 4.2], noticing that the Schatten \( \infty \) norm in that paper is exactly the spectral norm \( \|\cdot\|_2 \). Furthermore, we have strict inequality, that is \( YT\|_2 < \|g_0\|_{\infty} \), whenever the infimum of \( |g_0| \) is strictly bounded by \( \|g_0\|_{\infty} \), as it often occurs, including in our case.

Hence, \( \|YT_H\|_2 \) is uniformly bounded with respect to \( n \) and the proof is concluded.

By [5, Corollary 3] and Theorem 2.1, we know from Theorem 3.4 that the preconditioned matrix sequence \( \{P_H^{-1}YH\}_n \) has clustered eigenvalues around \( \pm 1 \), with a number of outliers independent of \( n \). Hence, the convergence is independent of the time steps, and we can then expect that MINRES converges rapidly in exact arithmetic with \( P_H \) as a preconditioner.

### 3.1.3 Eigenvalue analysis of \( (P_H^{-1}H)^TP_H^{-1}H \)

For a complete eigenvalue analysis, we in this subsection examine the preconditioned normal equation matrix \( (P_H^{-1}H)^TP_H^{-1}H \), even though we do not deploy the conjugate gradient method on normal equations (CGNE) in this work.

As for implementations, the product \( (P_H^{-1}H)^TP_H^{-1}Hv \) for any vector \( v \) can be computed effectively using the similar arguments in Section 3.1.1.

In the following result, we show that the eigenvalues of \( (P_H^{-1}H)^TP_H^{-1}H \) are clustered around 1 with outliers independent of the time step \( n \), which implies fast convergence of CGNE.

**Theorem 3.5.** Let \( T_H, P_H \in \mathbb{R}^{mn \times mn} \) be defined in (2) and (3), respectively. Then,

\[
(P_H^{-1}T_H)^TP_H^{-1}T_H = I_{mn} + \tilde{R}_H,
\]

where \( I_{mn} \) is the \( mn \) by \( mn \) identity matrix and \( \text{rank}(\tilde{R}_0) \leq m \).

**Proof.** Direct computations show that

\[
P_H^2 - T_H^TP_H = \begin{bmatrix}
O_m \\
& 
\ddots \\
& 
O_m \\
& 
A^2 \end{bmatrix} =: \tilde{R}_0,
\]

where \( \text{rank}(\tilde{R}_0) \leq m \). The matrix equation further leads to

\[
I_{mn} - T_HP_H^{-2}T_H^TP_H^{-1}T_H = I_{mn} - \tilde{R}_0^{-1}T_H^TP_H^{-1}T_H =: \tilde{R}_1,
\]

where \( \text{rank}(\tilde{R}_1) = \text{rank}(\tilde{R}_0) \leq m \).

We now consider the normal equation of \( P_H^{-1}YT_H \), namely

\[
(P_H^{-1}YT_H)^TP_H^{-1}YT_H = YT_HP_H^{-2}T_H^TP_H^{-1}YT_H = YT_H(I_{mn} - \tilde{R}_1)YT_H = I_{mn} - YT_H\tilde{R}_1YT_H =: \tilde{R}_H
\]

where \( \text{rank}(\tilde{R}_H) = \text{rank}(\tilde{R}_1) \leq m \).

Notice that every rank-one term in \( \tilde{R} \) can perturb at the same time one eigenvalue of 1. Therefore, by Theorem 3.5, there are at least \( n(m - 1) \) eigenvalues of the normal equation matrix are equal to 1, which implies rapid convergence of CGNE.
4 Extension to multistep methods

Our proposed preconditioning method can be easily extended for high-order time discretization schemes. Consider again (1), using an \( l \)-order backward difference scheme for time, we have the following all-at-once system

\[
\hat{T} \mathbf{u} = \hat{f}
\]

to solve for \( \mathbf{u} \), where

\[
\hat{T} = \begin{bmatrix}
A(0) & A(1) & \cdots & A(l) \\
A(1) & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots \\
A(l) & \cdots & A(1) & A(0)
\end{bmatrix}
\]

(14)

is a \( mn \) by \( mn \) multiple block Toeplitz matrix, which is generated by the matrix-valued function

\[
\hat{g}(x) = A(0) + A(1)e^{ix} + \cdots + A(l)e^{ilx},
\]

(15)

and \( \hat{f} \) is an appropriate vector resulted from the adopted discretization schemes. Note that the matrices \( A(k) \), \( k = 1, \ldots, l \), are composed of the mass matrix \( M_m \) and the stiffness matrix \( K_m \).

Our approach is to first permute (14) and obtain a symmetric (indefinite) matrix

\[
\mathcal{Y} \hat{T} = \begin{bmatrix}
A(l) & A(1) & A(0) \\
A(1) & \ddots & \ddots \\
\vdots & \ddots & \ddots \\
A(0) & \cdots & A(1) & A(l)
\end{bmatrix},
\]

(16)

and then construct a corresponding sine transform based preconditioner \( \hat{P} \) for it. We first compute the following matrix-valued function from (15)

\[
|\hat{g}(x)|^2 = A^2(0) + A^2(1) + \cdots + A^2(l)
\]

\[
+ (A(0)A(1) + A(1)A(2) + \cdots + A(l-1)A(l)) 2 \cos (x)
\]

\[
+ \cdots + (A(0)A(l)) 2 \cos (lx),
\]

where \( q_k, k = 1, \ldots, l \), are all matrix polynomials composed of \( A(k), k = 1, \ldots, l \).

Now, by expressing \( \cos (kx), k = 1, \ldots, l \), in terms of \( \cos (x) \), we can further rewrite \( |\hat{g}(x)|^2 \) as

\[
|\hat{g}(x)|^2 = \bar{q}_0(A) + \bar{q}_1(A) \cos (x) + \cdots + \bar{q}_l(A) \cos^l (x),
\]

where \( \bar{q}_k, k = 1, \ldots, l \), are certain matrix polynomials composed of \( A(k), k = 1, \ldots, l \).
We propose the following SPD preconditioner, which approximates the symbol $|\hat{g}|$ in the eigenvalue sense, for $\hat{Y}^T$:

$$
\hat{P} = \sqrt{I_n \otimes \bar{q}_0(A) + P_n \otimes \bar{q}_1(A) + \cdots + P_n^l \otimes \bar{q}_l(A)},
$$

(18)

where $P_n$ is the same matrix given by (10).

Note that

$$
\hat{P} = \sqrt{I_n \otimes U_0(\Lambda)U_m^T + P_n \otimes U_1(\Lambda)U_m^T + \cdots + P_n^l \otimes U_l(\Lambda)U_m^T}
$$

$$
= (S_n \otimes U_m)\sqrt{I_n \otimes \bar{q}_0(A) + D_n \otimes \bar{q}_1(A) + \cdots + D_n^l \otimes \bar{q}_l(A)}(S_n \otimes U_m)^T.
$$

Hence, the product $\hat{P}^{-1}v$ for any vector $v$ can be computed effectively using the similar three-step procedures in Section 3.1.1.

4.1 Eigenvalue analysis of $\hat{P}^{-1}\hat{Y}^T$

As before, we first introduce a block circulant matrix as an auxiliary for showing the eigenvalues of $\hat{P}^{-1}\hat{Y}^T$ are clustered.

$$
\hat{C} = \left[ \begin{array}{cccccc}
q_0(A) & q_1(A) & \cdots & q_l(A) & q_1(A) & \cdots \\
q_1(A) & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
q_l(A) & \ddots & \ddots & \ddots & \ddots & \ddots \\
q_1(A) & \ddots & \ddots & \ddots & \ddots & \ddots \\
q_1(A) & \ddots & \ddots & \ddots & \ddots & \ddots \\
\end{array} \right],
$$

where $q_k(A), k = 1, \ldots, l$, are the matrix polynomials given by (17).

By further introducing the block circulant preconditioner derived from (14) for $\hat{Y}^T$

$$
\hat{S} = \left[ \begin{array}{cccc}
A(0) & A(l) & \cdots & A(1) \\
A(1) & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & A(l) \\
A(l) & \cdots & A(1) & A(0) \\
\end{array} \right],
$$

we observe that $C$ can be rewritten as

$$
\hat{C} = \sqrt{\hat{S}^T\hat{S}} = \sqrt{\hat{S}\hat{S}^T}.
$$

(19)
The following proposition guarantees the effectiveness of $\hat{C}$ as a preconditioner for $\mathcal{Y}\hat{T}$, showing that the eigenvalues of $\{\hat{C}^{-1}\mathcal{Y}\hat{T}\}_n$ are clustered around $\pm 1$, which leads to fast convergence of MINRES.

**Proposition 4.1.** [32, Theorem 4] Let $\mathcal{Y}\hat{T}, \hat{C} \in \mathbb{R}^{mn \times mn}$ be defined in (16) and (19), respectively. Then,

$$\hat{C}^{-1}\mathcal{Y}\hat{T} = \hat{Q}_0 + \hat{R}_0,$$

where $\hat{Q}_0$ is symmetric and orthogonal, and $\text{rank}(\hat{R}_0) \leq lm$.

In addition, we require the following lemma and proposition for showing our main result.

**Lemma 4.2.** Let $\hat{C}, \hat{P} \in \mathbb{R}^{mn \times mn}$ be defined in (19) and (18), respectively. Then,

$$\text{rank}(\hat{C}^{2K} - \hat{P}^{2K}) \leq 2Klm$$

for some positive integer $K$ provided that $n > 2Klm$.

**Proof.** First, we observe from (17) that

$$T_{(n,m)}[|\hat{g}|^2] = T_{(n,m)}[q_0(A) + q_1(A)2 \cos(x) + \cdots + q_l(A)2 \cos(lx)]$$

$$= \begin{bmatrix} q_0(A) & q_1(A) & \cdots & q_l(A) \\ q_1(A) & \ddots & \cdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ q_l(A) & \cdots & \cdots & q_0(A) \end{bmatrix}.$$

Note that we also have

$$T_{(n,m)}[|\hat{g}|^2]$$

$$= T_{(n,m)}[\bar{q}_0(A) + \bar{q}_1(A) \cos(x) + \bar{q}_2(A) \cos^2(x) + \cdots + \bar{q}_l(A) \cos^l(x)]$$

$$= T_{(n,m)}[\bar{q}_0(A)] + T_{(n,m)}[\bar{q}_1(A) \cos(x)] + T_{(n,m)}[\bar{q}_2(A) \cos^2(x)] + \cdots + T_{(n,m)}[\bar{q}_l(A) \cos^l(x)]$$

$$= I_n \otimes \bar{q}_0(A) + T_{(n,1)}[\cos(x)] \otimes \bar{q}_1(A) + T_{(n,1)}[\cos^2(x)] \otimes \bar{q}_2(A) + \cdots + T_{(n,1)}[\cos^l(x)] \otimes \bar{q}_l(A)$$

$$= I_n \otimes \bar{q}_0(A) + T_{(n,1)}[\cos(x)] \otimes \bar{q}_1(A) + (T_{(n,1)}[\cos(x)]^2 + R(2)) \otimes \bar{q}_2(A) + \cdots + (T_{(n,1)}[\cos(x)]^l + R(l)) \otimes \bar{q}_l(A),$$

where $R(k), k = 2, \ldots, l$, are low rank matrices in the sense that $\text{rank}(R(k)) \leq 2(k - 1)$. 

14
Recalling from (18) that $\hat{P}^2 = I_n \otimes \eta_0(A) + P_n \otimes \eta_1(A) + \cdots + P_n^l \otimes \eta_l(A)$ and also note that $P_n = T_{(n,1)}[\cos(x)]$, we have

$$T_{(n,m)}[[\hat{g}]^2] = I_n \otimes \eta_0(A) + P_n \otimes \eta_1(A) + P_n \otimes \eta_2(A) + \cdots + (P_n^l + R(l)) \otimes \eta_l(A) = I_n \otimes \eta_0(A) + P_n \otimes \eta_1(A) + (P_n + R(2)) \otimes \eta_2(A) + \cdots + P_n^l \otimes \eta_l(A)$$

$$+ R(2) \otimes \eta_2(A) + \cdots + R(l) \otimes \eta_l(A).$$

One can further show by direct computations that $\hat{R}_1$ has the following structure

$$\hat{R}_1 = \begin{pmatrix}
* & \cdots & * \\
\vdots & \ddots & \vdots \\
* & \cdots & *
\end{pmatrix}$$

where * represents a nonzero entry, since such a block structure is determined by the last term $R(l) \otimes \eta_l(A)$. Namely, it is a block matrix with two blocks in the two corners and each block is of size $(l-1)m \times (l-1)m$.

We can now examine the structure of the matrix $\hat{C}^2 - \hat{P}^2$. By (19), we have

$$\hat{C}^2 - \hat{P}^2 = \hat{C}^2 - T_{(n,m)}[[\hat{g}]^2] + T_{(n,m)}[[\hat{g}]^2] - \hat{P}^2 =$$

$$= \begin{pmatrix}
q_1(A) & \cdots & q_1(A) \\
\ddots & \ddots & \ddots \\
q_l(A) & \cdots & q_l(A)
\end{pmatrix} + T_{(n,m)}[[\hat{g}]^2] - \hat{P}^2.$$

Thus, $\hat{C}^2 - \hat{P}^2$ is a block matrix with four $lm \times lm$ blocks in the four corners.

Similar to (12), by exploiting the simple structures of $\hat{C}^2 - \hat{P}^2$, we can show that for given positive integers $n_{\alpha}$ and $n_{\beta}$ the matrix $\hat{C}^{2n_{\alpha}}(\hat{C}^2 - \hat{P}^2)\hat{P}^{2n_{\beta}}$ is a block matrix with four blocks in its four corners and each block is of size $(n_{\alpha} + 1)lm \times (n_{\beta} + 1)lm$. Thus,

$$\hat{C}^{2K} - \hat{P}^{2K} = \sum_{i=0}^{K-1} (\hat{C}^{2K-2i} \hat{P}^{2i} - \hat{C}^{2K-2i-2} \hat{P}^{2i+2})$$

$$= \sum_{i=0}^{K-1} \hat{C}^{2K-2i-2}(\hat{C}^2 - \hat{P}^2) \hat{P}^{2i}.$$
is also a block matrix with four blocks in its four corners and each of them is of size $Klm \times Klm$, provided that $n > 2Klm$. Hence, we have $\text{rank}(\hat{C}^{2K} - \hat{P}^{2K}) \leq 2Klm$.

The following results, i.e. Proposition 4.3 and Theorem 4.4, follow using similar arguments for showing Preposition 3.3 and Theorem 3.4. Hence, the proofs are left to the readers.

**Proposition 4.3.** Let $\hat{C}, \hat{P} \in \mathbb{R}^{mn \times mn}$ be defined in (19) and (18), respectively. Then for any $\epsilon > 0$ there exists an integer $K$ such that for all $n > 2Klm$

$$\hat{C}^{-1} - \hat{P}^{-1} = \hat{E}_0 + \hat{R}_2,$$

where $\| \hat{E}_0 \|_2 \leq \epsilon$ and $\text{rank}(\hat{R}_2) \leq 2Klm$.

**Theorem 4.4.** Let $\hat{Y}^T, \hat{P} \in \mathbb{R}^{mn \times mn}$ be defined in (16) and (18), respectively. Then for any $\epsilon > 0$ there exists an integer $K$ such that for all $n > 2Km$

$$\hat{P}^{-1} \hat{Y}^T = \hat{Q} + \hat{E} + \hat{R},$$

where $\hat{Q}$ is both symmetric and orthogonal, $\| \hat{E} \|_2 \leq \epsilon$, and $\text{rank}(\hat{R}) \leq (2K + 1)lm$.

Since both $\hat{E}$ and $\hat{R}$ in Theorem 4.4 are symmetric, by [5, Corollary 3] and Theorem 2.1, we know that the preconditioned matrix sequence $\{\hat{P}^{-1} \hat{Y}^T\}_n$ has clustered eigenvalues around $\pm 1$ with number of outliers independent of $n$. Hence, the convergence is independent of the time steps, and we can then expect that MINRES converges rapidly in exact arithmetic with $\hat{P}$ as a preconditioner.

## 5 Numerical examples

In this section, we demonstrate the effectiveness of our proposed preconditioner. All numerical experiments are carried out using MATLAB on a HP EliteDesk 800 G5 Small Form Factor PC with Intel Core i7-9700 CPU @ 3.00GHz with 16GB RAM. The CPU time, which is denoted by “CPU” in the tables below, is estimated in seconds using the MATLAB build-in function `tic/toc`. All Krylov subspace solvers are implemented using the build-in functions on MATLAB, and “Iter” refers to the iteration number required for convergence. Furthermore, we choose a zero initial guess and a stopping tolerance of $10^{-6}$ based on the reduction in relative residual norms. Throughout all examples, we consider finite different methods with uniform spatial grids, which results in $M_m$ being the identity matrix and $K_m$ being diagonalized by the discrete sine transform. Note that in the examples “DoF” denotes the degree of freedom, and $C_H$ is the existing absolute value block circulant preconditioner proposed in [32].

### 5.1 Heat equations

**Example 5.1.** The first example is a one-dimensional problem of solving (1) with $\Omega = (0, 1)$, $u_0(x) = \sin^2(\pi x)$, $a(x) = 10^{-5}$, $g = 0$ and $f = 0$.

Table 1 shows the convergence results of MINRES when the Crank-Nicholson method is used for time. One can observe from the negative result that the MINRES iteration number with $C_H$ grows with $m$. In particular, we observe that the iteration numbers associated with $\mathcal{P}_H$ appear almost unchanged with both $n$ and $m$, i.e. mesh-independent convergence is achieved in effect. This improved number
Table 1: Convergence results with MINRES for Example 5.1 when $\theta = 0.5$ (the Crank-Nicolson method)

| MINRES | $C_H$ | $P_H$ |
|--------|-------|-------|
| $n \quad m + 1 \quad \text{DoF} \quad \text{Iter} \quad \text{CPU} \quad \text{Iter} \quad \text{CPU}$ |
| $2^8$ | 65280 | 59 | 0.67 | 16 | 0.14 |
| $2^9$ | 130816 | 61 | 1.31 | 16 | 0.30 |
| $2^{10}$ | 261888 | 62 | 3.04 | 16 | 0.69 |
| $2^{11}$ | 524032 | 62 | 6.18 | 16 | 1.45 |
| $2^9$ | 130560 | 60 | 1.31 | 17 | 0.32 |
| $2^9$ | 261632 | 61 | 2.61 | 17 | 0.62 |
| $2^{10}$ | 523776 | 62 | 6.20 | 17 | 1.44 |
| $2^{11}$ | 1048064 | 64 | 12.95 | 17 | 2.87 |
| $2^{10}$ | 261120 | 59 | 2.56 | 18 | 0.73 |
| $2^9$ | 523264 | 67 | 5.95 | 18 | 1.38 |
| $2^{10}$ | 1047552 | 67 | 13.67 | 18 | 3.21 |
| $2^{11}$ | 2096128 | 62 | 25.56 | 18 | 6.47 |
| $2^{11}$ | 522240 | 65 | 5.71 | 19 | 1.46 |
| $2^9$ | 1046528 | 68 | 12.37 | 19 | 2.92 |
| $2^{10}$ | 2095104 | 70 | 28.65 | 19 | 6.71 |
| $2^{11}$ | 4192256 | 70 | 57.031 | 19 | 13.28 |

Table 2: Convergence results with MINRES for Example 5.1 (BFD2)

| MINRES | $C_H$ | $P_H$ |
|--------|-------|-------|
| $n \quad m + 1 \quad \text{DoF} \quad \text{Iter} \quad \text{CPU} \quad \text{Iter} \quad \text{CPU}$ |
| $2^8$ | 65280 | 66 | 0.80 | 16 | 0.15 |
| $2^9$ | 130816 | 71 | 1.60 | 16 | 0.33 |
| $2^{10}$ | 261888 | 72 | 3.29 | 16 | 0.65 |
| $2^{11}$ | 524032 | 78 | 7.32 | 16 | 1.32 |
| $2^9$ | 130560 | 67 | 1.58 | 17 | 0.32 |
| $2^9$ | 261632 | 75 | 3.41 | 17 | 0.64 |
| $2^{10}$ | 523776 | 75 | 7.096 | 17 | 1.31 |
| $2^{11}$ | 1048064 | 77 | 14.68 | 17 | 2.73 |
| $2^{10}$ | 261120 | 68 | 3.22 | 18 | 0.75 |
| $2^9$ | 523264 | 77 | 7.34 | 18 | 1.50 |
| $2^{10}$ | 1047552 | 76 | 14.58 | 18 | 3.049 |
| $2^{11}$ | 2096128 | 84 | 32.13 | 18 | 6.11 |
| $2^{11}$ | 522240 | 80 | 7.43 | 19 | 1.53 |
| $2^9$ | 1046528 | 90 | 17.04 | 19 | 3.062 |
| $2^{10}$ | 2095104 | 85 | 32.44 | 19 | 6.22 |
| $2^{11}$ | 4192256 | 84 | 66.43 | 19 | 12.68 |

is in contrast with the existing preconditioner $C_H$. In Table 2, we observe similar convergence behaviours when the two-step backward-difference scheme (BFD2) is
Example 5.2. [32] The second example is a two-dimensional problem of solving (1) with $\Omega = (0,1) \times (0,1)$, $u_0(x,y) = x(x-1)y(y-1)$, $a(x,y) = 10^{-5}$, $g = 0$ and $f = 0$.

For this example, we adopt the backward Euler method and BFD2 in time for solving the equation and report the convergence results in Tables 3 and 4, respectively. While $C_H$ increases quickly in iteration number with the parameters for this ill-conditioned example, our proposed preconditioner $P_H$ significantly outperforms $C_H$.

Table 3: Convergence results with MINRES for Example 5.2 when $\theta = 1$ (the backward Euler method)

| MINRES | $C_H$ | $P_H$ |
|--------|-------|-------|
| $n$    | $m + 1$ | DoF | Iter | CPU | Iter | CPU |
| $2^5$  | $2^5$  | 30752 | 34 | 0.41 | 11 | 0.11 |
| $2^6$  | $2^6$  | 254016 | 48 | 2.43 | 11 | 0.56 |
| $2^7$  | $2^7$  | 2064512 | 73 | 25.95 | 13 | 4.38 |
| $2^8$  | $2^8$  | 16646400 | 80 | 339.43 | 14 | 47.03 |

Table 4: Convergence results with MINRES for Example 5.2 (BFD2)

| MINRES | $C_H$ | $P_H$ |
|--------|-------|-------|
| $n$    | $m + 1$ | DoF | Iter | CPU | Iter | CPU |
| $2^5$  | $2^5$  | 30752 | 42 | 0.33 | 11 | 0.090 |
| $2^6$  | $2^6$  | 254016 | 71 | 3.45 | 11 | 0.57 |
| $2^7$  | $2^7$  | 2064512 | 88 | 31.97 | 13 | 4.63 |
| $2^8$  | $2^8$  | 16646400 | 111 | 412.49 | 13 | 43.10 |
5.2 Wave equations

To illustrate that our proposed method is also applicable for other time-dependent equations, we in this subsection consider solving the following linear wave equation based on the same preconditioning strategy:

\[
\begin{cases}
    u_{tt}(x,t) = \Delta u(x,t) + f(x,t), & (x,t) \in \Omega \times (0,T], \\
    u = 0, & (x,t) \in \partial \Omega \times (0,T], \\
    u(x,0) = \psi_0, \quad u_t(x,0) = 0, & x \in \Omega.
\end{cases}
\]  

(20)

While there are many space-time discretization schemes for (20), we adopt here a first order two-step backwards finite difference scheme for time discretization, which was also used in [22]. For \(k = 2, \ldots, n\), we have in this case

\[
M_m \left( \frac{u_m^{(k-2)} - 2u_m^{(k-1)} + u_m^{(k)}}{\tau^2} \right) = -K_m u_m^{(k)} + f_m^{(k)}.
\]

where \(K_m \in \mathbb{R}^{m \times m}\) is again the second-order discrete matrix approximating the operator \(-\Delta\) in [20]. \(u_m^{(k)} = [u_m^{(k)}(1), \ldots, u_m^{(k)}(m)]^T\), and \(f_m^{(k)} = [f_m^{(k)}(1), \ldots, f_m^{(k)}(m)]^T\). In this case, we find the following equivalent all-at-once \(mn\)-by-\(mn\) (real) nonsymmetric block Toeplitz system \(\mathcal{T}_W u = f_W\)

\[
\mathcal{T}_W = \begin{bmatrix}
    M_m + \tau^2 K_m & -2M_m & M_m + \tau^2 K_m \\
    -2M_m & M_m & -2M_m & M_m + \tau^2 K_m \\
    \ddots & \ddots & \ddots & \ddots \\
    M_m & -2M_m & M_m + \tau^2 K_m
\end{bmatrix}
\]

and \(f_W = [(M_m + \tau^2 K_m)u_m^{(0)}, -M_m u_m^{(0)} + \tau^2 f_m^{(2)}, \tau^2 f_m^{(3)}, \ldots, \tau^2 f_m^{(n)}]^T\) is resulted from the used discretization schemes. Clearly, \(\mathcal{T}_W\) is generated by the matrix-valued function \(g_{\text{wave}}(x) = A(0) + A(1)e^{ix} + A(2)e^{2ix}\)

with \(A(0) = M_m + \tau^2 K_m\), \(A(1) = -2M_m\), and \(A(2) = M_m\).

For \(Y \mathcal{T}_W\), using (18) we propose the preconditioner \(\mathcal{P}_W = \sqrt{\mathcal{P}_W^2}\), where

\[
\mathcal{P}_W^2 = I_n \otimes (A_0^2 + A_1^2 + A_2^2 - 2A_0 A_2) + P_n \otimes 2(A_0 A_1 + A_1 A_2) + P_n \otimes 4A_0 A_2.
\]

Example 5.3. [22] This example is a one-dimensional problem for solving (20) with \(\Omega = (0,1), \psi_0(x) = \chi_{3/8,5/8}(x) \cos^2(4\pi(x - 1/2)), \) and \(f = 0\). Note that \(\chi_X\) is the indicator function on the set \(X\).

Tables 5 and 6 show the MINRES convergence results when BFD2 and the central difference scheme adopted in [22] for time are used, respectively. When the central difference scheme is used, the existing block circulant preconditioner \(\mathcal{C}_W\) that we compare against is the one proposed in [22] Eq. (2.20)]. Again, our proposed preconditioner works well for this ill-conditioned example, while \(\mathcal{C}_W\) fails to accelerate convergence.

In both Figures 1 and 2 we observe the expected clustered eigenvalues around \(\pm 1\) when the preconditioners are used. Notice that the severe ill-conditioning of the original matrix is improved by \(\mathcal{P}_W\). Namely, there are fewer near-zero eigenvalues present compared with the spectrum resulted by \(\mathcal{C}_W\), which indicates the better performance of \(\mathcal{P}_W\) over \(\mathcal{C}_W\).
Table 5: Convergence results with MINRES for Example 5.3 (BFD2)

| MINRES | $C_W$ | $P_W$ |
|--------|-------|-------|
| $n$    | $m+1$ | DoF   | Iter | CPU  | Iter | CPU  |
| 2$^7$  | 2$^7$  | 16256 | 190  | 0.36 | 30   | 0.058 |
| 2$^8$  | 2$^8$  | 65280 | 493  | 5.35 | 33   | 0.27  |
| 2$^9$  | 2$^9$  | 261632| >500 | -    | 33   | 1.11  |
| 2$^{10}$ | 2$^{10}$ | 1047552 | -   | -    | 37   | 5.80  |

Table 6: Convergence results with MINRES for Example 5.3 (the central difference scheme)

| MINRES | $C_W$ | $P_W$ |
|--------|-------|-------|
| $n$    | $m+1$ | DoF   | Iter | CPU  | Iter | CPU  |
| 2$^7$  | 2$^7$  | 16256 | 190  | 0.36 | 30   | 0.058 |
| 2$^8$  | 2$^8$  | 65280 | 493  | 5.35 | 33   | 0.27  |
| 2$^9$  | 2$^9$  | 261632| >500 | -    | 33   | 1.11  |
| 2$^{10}$ | 2$^{10}$ | 1047552 | -   | -    | 37   | 5.80  |

Example 5.4. In the last example, we consider solving \[ (20) \] with $\Omega = (0,1) \times (0,1)$ and $\psi_0(x,y) = x(x-1)y(y-1)$ and $f = \frac{x(x-1)(y(y-1))}{t+1} - 2((t+1)\ln (t+1) - t + 1)(x(x-1) + y(y-1))$. 

20
Table 7 shows the MINRES convergence results when BFD2 is applied. While it is observed that our preconditioner $\mathcal{P}_W$ in this badly ill-conditioned case grows with both $n$ and $m$ in this case, it is nevertheless more effective than $\mathcal{C}_W$. We stress that the severity of ill-conditioning of the original linear system mainly comes from both the spatial and temporal discretization schemes for the underlying equation. In addition to effective preconditioning, one remedy is to develop better discretization schemes in the first place for both space and time, which would be a potential research direction in the next stage.

In Table 8 where the central difference method is used, we observe that MINRES with $\mathcal{C}_W$ fails to converge for all choices of $(n, m)$ compared, while $\mathcal{P}_W$ leads to rapid convergence.

### Table 7: Convergence results with MINRES for Example 5.4 (BFD2)

| $n$  | $m + 1$ | DoF      | Iter | CPU  | $n$  | $m + 1$ | DoF      | Iter | CPU  |
|------|---------|----------|------|------|------|---------|----------|------|------|
| $2^5$| $2^5$   | 30752    | 44   | 0.34 | $2^6$| $2^6$   | 254016   | 79   | 3.84 |
| $2^6$| $2^6$   | 2064512  | 166  | 58.60| $2^7$| $2^7$   | 16646400 | >200 | -    |
| $2^7$| $2^7$   | 2064512  | 166  | 58.60| $2^8$| $2^8$   | 16646400 | >200 | -    |

### Table 8: Convergence results with MINRES for Example 5.4 (the central difference scheme)

| $n$  | $m + 1$ | DoF      | Iter | CPU  | $n$  | $m + 1$ | DoF      | Iter | CPU  |
|------|---------|----------|------|------|------|---------|----------|------|------|
| $2^5$| $2^5$   | 30752    | -    | -    | $2^6$| $2^6$   | 254016   | -    | -    |
| $2^6$| $2^6$   | 2064512  | -    | -    | $2^7$| $2^7$   | 2064512  | -    | -    |
| $2^7$| $2^7$   | 16646400 | -    | -    | $2^8$| $2^8$   | 16646400 | -    | -    |

### 6 Conclusions

We have developed in this work a sine transform based preconditioning method which can be used for solving a wide range of time-dependent PDEs. Namely, our proposed preconditioner can be applied for a large class of symmetrized all-at-once system $\mathcal{Y}^T \mathcal{F}$ resulted from discretizing the underlying equation. The method is generic, and can be used with high-order discretization schemes for time.

We have adopted the Krylov subspace solver of MINRES by exploiting the symmetry of the permuted matrix. In particular, we emphasize that our sine transform based preconditioner $\hat{P}$ can be seen as an optimal or quasi optimal preconditioner, which is both symmetric positive definite and efficiently implemented, according to our previous work on the spectral distribution of symmetrized Toeplitz matrix sequences [15]. We observe that a quasi optimal behavior is obtained in the case of
multilevel coefficient matrices, which is a good result given the theoretical barriers proven in [38, 39].

Also, specifically designed for MINRES, our preconditioner $\hat{P}$ consistently outperforms the existing block circulant preconditioner $\hat{C}$ in both iteration counts and CPU times as shown in each numerical example. It is observed that $\hat{P}$ achieves rapid convergence in both ill-conditioned case and well-conditioned case.

Our preconditioning technique utilizes the fast diagonalizability of the Laplacian matrix, which relies mainly on the uniform spatial grid setting. We however emphasize that such an uniform grid assumption is a common setting in the all-at-once preconditioning context, as with many existing works such as [28, 42]. Along this line, it would be a direction for future research to develop efficient preconditioning methods when the physical domain is irregular - in this setting the theory of generalized locally Toeplitz sequences could be exploited for the spectral and convergence analysis [36, 2].

For another future work, it would be interesting to combine the proposed symmetrization MINRES solver with the block $\epsilon$-circulant preconditioning technique [27, 30] which has only shown applicable for GMRES. Such a combination would further advance the pioneering block circulant preconditioner $\hat{C}$ (cooperated with MINRES) originally proposed in [32], which is still at an early stage of development.

Acknowledgments

The work of Sean Hon was supported in part by the Hong Kong RGC under grant 22300921, a start-up allowance from the Croucher Foundation, and a Tier 2 Start-up Grant from Hong Kong Baptist University. The work of Stefano Serra-Capizzano was supported in part by INDAM-GNCS.

References

[1] Nikos Barakitis, Sven-Erik Ekstrom, and Paris Vassalos. Preconditioners for fractional diffusion equations based on the spectral symbol. arXiv:1912.13304, 2019.

[2] Giovanni Barbarino. A systematic approach to reduced GLT. BIT Numerical Mathematics, 2021.

[3] Michele Benzi and Gene H. Golub. Bounds for the entries of matrix functions with applications to preconditioning. BIT Numerical Mathematics, 39(3):417–438, 1999.

[4] Dario Bini and Milvio Capovani. Spectral and computational properties of band symmetric Toeplitz matrices. Linear Algebra and Its Applications, 52/53:99–126, 1983.

[5] Jan H. Brandts and Ricardo Reis da Silva. Computable eigenvalue bounds for rank-$k$ perturbations. Linear Algebra and Its Applications, 432(12):3100–3116, 2010.

[6] Stefano Serra Capizzano and Paolo Tilli. On unitarily invariant norms of matrix-valued linear positive operators. Journal of Inequalities and Applications, 7(3):309–330, 2002.

[7] Raymond H. Chan and K. N.G. Michael. Conjugate gradient methods for Toeplitz systems. SIAM Review, 38(3):427–482, 1996.
[8] Tony F. Chan. An Optimal Circulant Preconditioner for Toeplitz Systems. *SIAM Journal on Scientific and Statistical Computing*, 9(4):766–771, 1988.

[9] Federico Danieli and Andrew J. Wathen. All-at-once solution of linear wave equations. *Numerical Linear Algebra with Applications*, page e2386, 2021.

[10] Fabio Di Benedetto. Analysis of preconditioning techniques for ill-conditioned Toeplitz matrices. *SIAM Journal on Scientific Computing*, 16(3):682–697, 1995.

[11] Fabio Di Benedetto. Solution of Toeplitz normal equations by sine transform based preconditioning. *Linear Algebra and Its Applications*. 285(1-3), 229–255, 1998.

[12] V. A. Dobrev, Tz Kolev, N. A. Petersson, and J. B. Schroder. Two-level convergence theory for multigrid reduction in time (MGRIT). *SIAM Journal on Scientific Computing*, 39(5):S501–S527, 2017.

[13] Marco Donatelli, Mariarosa Mazza, and S. Serra-Capizzano. Spectral analysis and structure preserving preconditioners for fractional diffusion equations. *Journal of Computational Physics*, 307:262–279, 2016.

[14] R D Falgout, S Friedhoff, Tz. V Kolev, S P MacLachlan, and J B Schroder. Parallel Time Integration with Multigrid. *SIAM Journal on Scientific Computing*, 36(6):C635–C661, 2014.

[15] Paola Ferrari, Isabella Furci, Sean Hon, Mohammad Ayman Mursaleen, and Stefano Serra-Capizzano. The eigenvalue distribution of special 2-by-2 block matrix-sequences with applications to the case of symmetrized Toeplitz structures. *SIAM Journal on Matrix Analysis and Applications*, 40(3):1066–1086, 2019.

[16] Martin J Gander. 50 Years of Time Parallel Time Integration. In Thomas Carraro, Michael Geiger, Stefan Körkel, and Rolf Rannacher, editors, *Multiple Shooting and Time Domain Decomposition Methods*, pages 69–113, Cham, 2015.

[17] Martin J Gander, Laurence Halpern, Juliet Ryan, and Thuy Thi Bich Tran. A Direct Solver for Time Parallelization. In Thomas Dickopf, Martin J Gander, Laurence Halpern, Rolf Krause, and Luca F Pavarino, editors, *Domain Decomposition Methods in Science and Engineering XXII*, pages 491–499, Cham, 2016.

[18] Martin J Gander and Martin Neumüller. Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems. *SIAM Journal on Scientific Computing*, 38(4):A2173–A2208, 2016.

[19] Martin J Gander and Stefan Vandewalle. Analysis of the Parareal Time-Parallel Time-Integration Method. *SIAM Journal on Scientific Computing*, 29(2):556–578, 2007.

[20] Carlo Garoni and Stefano Serra-Capizzano. *Generalized locally Toeplitz sequences: Theory and applications*, volume 1. Springer, Cham, 2017.

[21] Carlo Garoni and Stefano Serra-Capizzano. *Generalized locally Toeplitz sequences: Theory and applications*, volume 2. Springer, Cham, 2018.

[22] Anthony Goddard and Andy Wathen. A note on parallel preconditioning for all-at-once evolutionary PDEs. *Electronic Transactions on Numerical Analysis*, 51:135–150, 2019.
[23] Sean Hon. Optimal block circulant preconditioners for block Toeplitz systems with application to evolutionary PDEs. *Journal of Computational and Applied Mathematics*, page 113965, 2021.

[24] Sean Hon, Mohammad Ayman Mursaleen, and Stefano Serra-Capizzano. A note on the spectral distribution of symmetrized Toeplitz sequences. *Linear Algebra and Its Applications*, 579(2-3):32–50, 2019.

[25] Sean Hon, Stefano Serra-Capizzano, and Andy Wathen. Band-Toeplitz preconditioners for ill-conditioned Toeplitz systems. *BIT Numerical Mathematics*, 2021.

[26] G Horton and S Vandewalle. A Space-Time Multigrid Method for Parabolic Partial Differential Equations. *SIAM Journal on Scientific Computing*, 16(4):848–864, 1995.

[27] Xue-lei Lin and Michael Ng. An all-at-once preconditioner for evolutionary partial differential equations. *SIAM Journal on Scientific Computing*, 43(4):A2766–A2784, 2021.

[28] Xue-lei Lin, Michael K Ng, and Yajing Zhi. A parallel-in-time two-sided preconditioning for all-at-once system from a non-local evolutionary equation with weakly singular kernel. *Journal of Computational Physics*, 434:110221, 2021.

[29] Jacques Louis Lions, Yvon Maday, and Gabriel Turinici. A “parareal” in time discretization of PDE’s. *Comptes rendus de l’Académie des sciences. Série I, Mathématique*, 332(7):661–668, 2001.

[30] Jun Liu and Shu Lin Wu. A fast block α-circulant preconditioner for all-at-once systems from wave equations. *SIAM Journal on Matrix Analysis and Applications*, 41(4):1912–1943, 2021.

[31] Eleanor McDonald, Sean Hon, Jennifer Pestana, and Andy Wathen. Preconditioning for nonsymmetry and time-dependence. In *Lecture Notes in Computational Science and Engineering*, volume 116, pages 81–91. Springer International Publishing, 2017.

[32] Eleanor McDonald, Jennifer Pestana, and Andy Wathen. Preconditioning and iterative solution of all-at-once systems for evolutionary partial differential equations. *SIAM Journal on Scientific Computing*, 40(2):A1012–A1033, 2018.

[33] Michael K. Ng. *Iterative Methods for Toeplitz Systems*. Numerical Mathematics and Scientific Computation. Oxford University Press, New York, 2004.

[34] Michael K. Ng and Jianyu Pan. Approximate inverse circulant-plus-diagonal preconditioners for Toeplitz-plus-diagonal matrices. *SIAM Journal on Scientific Computing*, 32(3):1442–1464, 2010.

[35] Stefano Serra-Capizzano. Superlinear PCG methods for symmetric Toeplitz systems. *Mathematics of Computation*, 68(226):793–803, 1999.

[36] Stefano Serra-Capizzano. The GLT class as a generalized Fourier analysis and applications. *Linear Algebra and Its Applications*, 419(1), 180–233, 2006.

[37] Stefano Serra-Capizzano. Toeplitz preconditioners constructed from linear approximation processes. *SIAM Journal on Matrix Analysis and Applications*, 20(2):446–465, 1999.

[38] Stefano Serra-Capizzano and Eugene E Tyrtyshnikov. Any circulant-like preconditioner for multilevel matrices is not superlinear. *SIAM Journal on Matrix Analysis and Applications*, 21(2):431–439, 1999.
[39] Stefano Serra-Capizzano and Eugene E Tyrtyshnikov. How to prove that a preconditioner cannot be superlinear. *Mathematics of Computation*, 72(243):1305–1316, 2003.

[40] Gilbert Strang. A Proposal for Toeplitz Matrix Calculations. *Studies in Applied Mathematics*, 74(2):171–176, 1986.

[41] Andy Wathen. Preconditioning. *Acta Numerica*, 24:329–376, 2015.

[42] Shu-Lin Wu and Tao Zhou. Parallel implementation for the two-stage SDIRK methods via diagonalization. *Journal of Computational Physics*, 428:110076, 2021.