STABILITY IMPLIES ROBUST CONVERGENCE OF A CLASS OF DIAGONALIZATION-BASED ITERATIVE ALGORITHMS

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Abstract. Solving wave equations in a time-parallel manner is challenging, and the algorithm based on the block α-circulant preconditioning technique has shown its advantage in many existing studies (where $\alpha \in (0,1)$ is a free parameter). Considerable efforts have been devoted to exploring the spectral radius of the preconditioned algebraic system. Then, we need $N$ time steps, which requires to compute the numerical solution at discrete time levels one by one. In this paper, we only consider the implicit time-integrator. Our analysis works for all one-step time-integrators and two exemplary classes of two-step time-integrators: the parameterized Numerov methods and the parameterized two-stage hybrid methods. The main conclusion is that the global error satisfies $\|\text{err}^{k+1}\|_W \leq \frac{\alpha}{1-\alpha} \|\text{err}^k\|_W$ provided that the time-integrator is stable, where $k$ is the iteration index and for any vector $v$ the norm $\|v\|_W$ is defined by $\|v\|_W = \|Wv\|_2$ with $W$ being a matrix depending on the space discretization matrix only. Even though we focus on wave equations in this paper, the proposed argument is directly applicable to other evolution problems.

Key words. parallel-in-time, wave equations, α-circulant preconditioner, convergence analysis, stability

AMS subject classifications. 65M55, 65M12, 65M15, 65Y05

1. Introduction. We are interested in fast algorithm for approximately solving the wave equation

$$\partial_t u(x,t) = \Delta u(x,t) + f(x,t), \quad (x,t) \in \Omega \times (0,T),$$

(1.1)

supplied with suitable boundary conditions, where $\Delta$ is the Laplacian operator and $\Omega \in \mathbb{R}^d$ with $d = 1, 2, 3$. The initial conditions for (1.1) are $u(x,0) = u_0(x)$ and $\partial_t u(x,0) = v_0(x)$. Suppose $A \in \mathbb{R}^{N_x \times N_x}$ is the matrix of the discrete Laplacian, obtained via finite-difference or finite-element methods (in this case $A = M^{-1}K$ with $M$ and $K$ being respectively the mass and stiff matrices). Then, we arrive at the following spatially semi-discrete system in matrix form:

$$U''(t) + AU(t) = F(t), \quad t \in (0,T),$$

(1.2)

together with the initial conditions $U(0) = \Phi_0$ and $U'(0) = \Phi_1$, where $U(t)$ is a column vector containing the approximate values of $u(x,t)$ over all the grid nodes of the spatial mesh and similar explanation goes to other symbols. In this paper we only consider the implicit time-integrators, which requires to compute the numerical solution at discrete time levels one by one and each step consists of solving an algebraic system. Suppose it takes $\tau$ seconds to solve the algebraic system. Then, we need $N_t \tau$ seconds in total for crossing $N_t$ time steps. This will be a serious problem if $N_t$ is large and/or $\tau$ is large.

The research toward reducing the overall computation time via parallelization across time steps is a hot topic in the recent twenty years, since the appearance of the parareal algorithm in 2001 [25]. The parareal algorithm (and its several variants, e.g., the PFFAST algorithm [7] and the MGRiT algorithm [9]) works very well for strongly dissipative problems, while the convergence rate continuously deteriorates as the dissipativity becomes weaker. Efforts devoted to modifying the parareal algorithm to make it suitable for wave propagation problems can be found in many places [2, 4, 6, 8, 10, 11, 30–32], but the complicated modification often leads to...
degradation of efficiency or limited applicability. A most recent work in this direction is [16], where new parareal algorithm keeps the simplicity of the original algorithm and has provable estimate of the convergence factor smaller than $\frac{2\alpha N_t}{1+\alpha}$ for the wave equation (1.1), where $N_t$ is the number coarse time points and $\alpha \in (0, 1)$ is a free parameter. However, the dependence on $N_t$ will be a problem, because for large $N_t$ we have to use a very small $\alpha$ to yield fast convergence and a small $\alpha$ may cause serious roundoff error in practical implementation (a huge roundoff error in turn affects the convergence rate).

An alternative approach is to use the diagonalization technique proposed by Maday and Ronquist in 2008 [29]. The basic idea is as follows. We first formulate the space-time discretization into an all-at-once system and then diagonalize the time stepping matrix and solve all time steps in parallel. (The space discrete matrix is kept unchanged.) Such a technique was first used in [14] for the wave equation (1.1). The concrete algorithm lies in using the geometrically increasing time step-sizes $\{\Delta t_n = \mu^{n-1}\Delta t_1\}_{n=1}^{N_t}$ with some parameter $\mu > 1$ to make the time discretization matrix diagonalizable. The algorithm is directly parallel (i.e., non-iterative), but to balance the roundoff error arising from the diagonalization procedure and the discretization error the quantity $N_t$ can not be large ($N_t = 20 \sim 25$ in practice).

To overcome the restriction on step size $N_t$, the diagonalization technique was used in an iterative fashion [17, 18, 23, 26–28]. These iterative algorithms use a uniform step-size and have a uniform convergence rate for any value of $N_t$. The algorithm in [17, 28] lies in constructing a block circulant preconditioner and then solving the all-at-once system by some Krylov subspace solver. For heat equations, this preconditioner leads to rapid convergence for the GMRES method, but for the wave equation (1.1) GMRES converges very slowly. In [18, 23, 26, 27], a block $\alpha$-circulant preconditioner is proposed, which is a generalized version of the preconditioner studied in [17, 28]. Let $K$ be the all-at-once matrix specified by the space and time discretizations and $P_\alpha$ be the block $\alpha$-circulant preconditioner. Then, for some special time-integrators (e.g., the implicit Euler method [26, 27], the implicit leap-frog method [23], the two-step BDF method [18] and the two-stage singly diagonal implicit Runge-Kutta (SDIRK) method [34]) it was shown in these work

$$\rho(I - P_\alpha^{-1}K) \leq \frac{\alpha}{1 - \alpha}, \quad \alpha \in (0, 1).$$

(1.3)

Hence, we can solve the all-at-once system

$$K u = b,$$

(1.4)

by a preconditioned stationary fixed-point iteration

$$u^{k+1} = u^k - P_\alpha^{-1}(Ku^k - b), \quad k = 0, 1, \ldots$$

(1.5)

Thanks to the property of the $\alpha$-circulant matrices (see, e.g., [1, Lemma 2.1]), we can make a block Fourier diagonalization for the preconditioner $P_\alpha$ and this allows to compute $P_\alpha^{-1}(Ku^k - b)$ in (1.5) highly parallel for all time levels. The details will be explained in Section 2. The convergence of (1.5) was carefully justified via analyzing iteration matrix $I - P_\alpha^{-1}K$ in [17, 18, 26–28] for parabolic problems and in [15, 23] for the wave equation (1.1). The analysis in these pioneer works is rather technical and heavily depends on the special property of the time-integrator (e.g., the sparsity, Toeplitz structure and diagonal dominance of the time-discretization matrix [18, 23, 26–28, 33, 34]).

The iterative algorithm (1.5) however does not always converges rapidly and it actually depends on the used time-integrator. To illustrate this, we consider the well-known 4th-order Numerov method [20] as an example:

$$\frac{U_{n+1} - 2U_n + U_{n-1}}{\Delta t^2} + A \frac{U_{n+1} + 10U_n + U_{n-1}}{12} = F_n := \frac{F_{n+1} + 10F_n + F_{n-1}}{12},$$

(1.6)
where \( n = 1, 2, \ldots, N_t \) with \( N_t = T/\Delta t - 1 \). It is a two-step methods and hence requires two starting values \( U_0 = \Phi_0 \) and \( U_1 \) (without loss of generality we assume here and hereafter that \( U_1 \) is already available). We can either get \( U_1 \) via Taylor expansion of \( U(t) \) at \( t = \Delta t \) as in [24] or some one-step method.). Let \( \mathbf{u} = (U_2^T, \ldots, U_{N_t+1}^T)^T \), \( K = B_1 \otimes I_x + B_2(\gamma) \otimes \Delta t^2 A \) and \( P_\alpha = C_1(\alpha) \otimes I_t + C_2(\alpha, \gamma) \otimes \Delta t^2 A \) with

\[
B_1 = \begin{bmatrix}
1 & -2 & 1 \\
1 & -2 & 1 \\
1 & -2 & 1
\end{bmatrix},
\]

\[
B_2(\gamma) = \begin{bmatrix}
\gamma & 1 - 2\gamma & \gamma \\
\gamma & 1 - 2\gamma & \gamma \\
\gamma & 1 - 2\gamma & \gamma
\end{bmatrix},
\]

\[
C_1(\alpha) = \begin{bmatrix}
1 & \alpha & -2\alpha \\
1 & \alpha & -2\alpha \\
1 & \alpha & -2\alpha
\end{bmatrix},
\]

\[
C_2(\alpha, \gamma) = \begin{bmatrix}
1 - 2\gamma & \gamma & \alpha \gamma \\
1 - 2\gamma & \gamma & \alpha \gamma \\
1 - 2\gamma & \gamma & \alpha \gamma
\end{bmatrix}.
\]

Then, we can represent the 4-th order Numerov method (1.6) as the all-at-once system (1.4) with a suitable right hand-side term \( \mathbf{b} \) and the parameter \( \gamma = \frac{1}{\Delta t} \). Hence the preconditioned iterative scheme can be written as (1.5). The parameterized Numerov method with general \( \gamma \) which will be addressed in Section 3.1.

In Figure 1.1 (left), we present the spectrum \( \sigma(I - P_\alpha^{-1}K) \) in a 2D case with various step size \( \Delta t \), where we apply the finite difference method with a fixed mesh size \( \Delta x = \frac{1}{40} \). We see that the spectral radius of the iterative matrix satisfies (1.3) when \( \Delta t = \frac{1}{40} \), while for \( \Delta t = \frac{1}{40} \) the estimate (1.3) does not hold because many eigenvalues lie outside the circle. In Figure 1.1 (right), we plot the error \( \| \mathbf{u}^k - \mathbf{u} \|_2 \) of the iteration (1.5) and the convergence behavior is consistent with the spectrum very well.

In this paper, we aim to answer the question: under what conditions of the time-integrator the iterative algorithm (1.5) converges rapidly and robustly? Instead of exploring the spectrum of the iterative matrix as people did in many pioneer works [18,23,26,27], we will examine error of the preconditioned iteration directly, and in particular we will prove

\[
\| \text{err}^{k+1} \|_{W, 2} \leq \frac{\alpha}{1 - \alpha} \| \text{err}^k \|_{W, 2},
\]

provided that the time-integrator is stable, where \( \text{err}^k \) is the error at the \( k \)-th iteration. Here and hereafter, for any vector \( \mathbf{v} \) with suitable length the norm \( \| \cdot \|_{w, 2} \) is defined by \( \| \mathbf{v} \|_{W, 2} = \| \mathbf{W} \mathbf{v} \|_2 \), where \( \mathbf{W} \) is a matrix depending on the space discretization matrix \( A \) only. This conclusion well explains the results obtained in [15,16,18,26,27], because the time-integrators used there are unconditionally stable. If the time-integrator is conditionally stable, this conclusion can be used to select the space and time step-sizes; we will discuss this point for Figure 1.1 on the right in Remark 3.2. Note that the convergence of a PinT algorithm for parabolic equations was analyzed in [33] via applying the stability of BDF schemes. The current work provides a more systematic argument showing the relation between stability of time-integrators and the convergence of the iterative solver (1.5). Even though we focus on wave equations in this paper, the proposed argument is directly applicable to other evolution problems.

The rest of this paper is summarized as follows. In Section 2 we prove the convergence estimate (1.8) for a general one-step time-integrator under the stability condition. Note that the one-step time-integrator to the wave equation (1.1) usually requires an order reduction to rewrite the equation as a first-order system, and as a result this doubles the storage complexity
at each time point. In Section 3 we prove (1.8) for two class of representative two-step time-integrators which are directly applied to (1.1) without an order reduction. Our numerical results are given in Section ?? by considering the hanging string problem and the Brusselator reaction with diffusion. The former is a second-order ODE system arising from mechanics and the latter is a typical nonlinear stiff PDE with first-order temporal derivative. We will validate (1.8) for the two-step time-integrator by using the hanging string problem and for the one-step Runge-Kutta method by using the Brusselator equation. We conclude this paper in Section 4.

2. One-step time-integrators. In this section, we provide a rigorous proof of (1.8) for any one-step time-integrators, which includes the trapezoidal rule and the Runge-Kutta method. In this case, we first reduce the second-order differential equation (1.2) to a coupled first-order system as

\[ w'(t) + Qw(t) = \bar{F}(t), \quad Q := \begin{bmatrix} 0 & -I_x \\ A & -I_x \end{bmatrix}, \]

(2.1)
where \( w(t) = (U^\top(t), V^\top(t))^\top \) with \( V(t) \) being an auxiliary function and \( \bar{F}(t) = (0, F^\top(t))^\top \). Then a one-step time-integrator applied to (2.1) can be written as the form:

\[
w_{n+1} = \mathcal{R}(\Delta tQ)w_n + \Delta tg_n, \quad n = 0, 1, \ldots, N_t - 1,
\]

where \( \mathcal{R}(z) \) is the stability function of the time-integrator, and \( g_n \) is a suitable term specified by \( \bar{F}(t) \) and the time-integrator under consideration.

For example, the trapezoidal rule (Crank-Nicolson scheme) can be written as

\[
\mathcal{R}(\Delta tQ) = (I_x + \Delta tQ/2)^{-1}(I_x - \Delta tQ/2), \quad g_n = (I_x + \Delta tQ/2)^{-1}\bar{F}_n + \bar{F}_{n+1}/2.
\]

Moreover, for the 4th-order Gauss Runge-Kutta method, \( \mathcal{R}(\Delta tQ) \) and \( g_n \) should be

\[
\mathcal{R}(\Delta tQ) = (I_x + \Delta tQ/2 + (\Delta tQ)^2/12)^{-1}(I_x - \Delta tQ/2 + (\Delta tQ)^2/12),
\]

\[
g_n = (b_s \otimes I_x - \Delta t(b_s \otimes Q)(I_x \otimes I_x + \Delta t\Phi_s \otimes Q)^{-1}(\Phi_s \otimes I_x))[\bar{F}^\top(t_n + c_1\Delta t), \bar{F}^\top(t_n + c_2\Delta t)\]^\top,
\]

where \( (\Phi_s, b_s, c_s) \) is the Butcher’s tabula used to specify an \( s \)-stage RK method. In particular, for the 4th-order Gauss RK method, it holds

\[
\Phi_s = \begin{bmatrix}
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} - \frac{\sqrt{3} \pi}{6} \\
\frac{1}{3} + \frac{\sqrt{3} \pi}{6} & \frac{1}{3} & \frac{1}{3}
\end{bmatrix}, \quad b_s = \begin{bmatrix}
1 & 1 & 1 \\
0 & 0 & 1
\end{bmatrix}, \quad c_s = \begin{bmatrix}
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} - \frac{\sqrt{3} \pi}{6} \\
\frac{1}{3} + \frac{\sqrt{3} \pi}{6} & \frac{1}{3} & \frac{1}{3}
\end{bmatrix}.
\]

The matrix \( \mathcal{R}(\Delta tQ) \) is just a mathematical tool to perform the convergence analysis and in practice we do not have to form it. This will be clear from the description of the diagonalization technique in the following.

Let \( w = (w_1^\top, \ldots, w_{N_t}^\top)^\top, \mathcal{K} = I_t \otimes I_x + B \otimes \mathcal{R}(\Delta tQ) \) and \( \mathcal{P}_\alpha = I_t \otimes I_x + C(\alpha) \otimes \mathcal{R}(\Delta tQ) \) with

\[
B = \begin{bmatrix}
0 & 1 & 0 & \cdots & 0 \\
1 & 0 & 1 & \cdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\cdots & \cdots & \cdots & \ddots & \cdots \\
1 & 0 & \cdots & \cdots & 0
\end{bmatrix}, \quad C(\alpha) = \begin{bmatrix}
0 & 0 & -\alpha \\
-1 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
\cdots & \cdots & \ddots & \cdots \\
-1 & 0
\end{bmatrix}.
\]

Then, we can represent (2.2) as \( \mathcal{K}w = b \) with \( b = ((\mathcal{R}(\Delta tQ)w_0 + \Delta t g_0)^\top, \Delta t g_1^\top, \ldots, \Delta t g_{N_t-1}^\top)^\top \).

Then, similar to (1.5) we solve this system via the following preconditioned iteration

\[
w^{k+1} = w^k - \mathcal{P}_\alpha^{-1}(\mathcal{K}w^k - b), \quad k = 0, 1, \ldots
\]

For each iteration of (2.4), the major computation is twofold. The first is to compute the residual \( r^k = \mathcal{K}w^k - b \). In the parallel circumstance, the \( N_t \) subvectors \( \{w_{n,k}\}_{n=1}^{N_t} \) are stored in the \( N_t \) cores and thus the subvectors \( \{r_{n,k}\}_{n=1}^{N_t} \) of the residual \( r^k \) can be constructed simultaneously. The second major cost is to compute \( \mathcal{P}_\alpha^{-1}r^k \) and this computation is based on the diagonalization technique addressed as follows.

Let \( \Phi = \frac{1}{\sqrt{N_t}} \sum_{i=1}^{N_t} w_{i1}w_{i2} \) (with \( i = \sqrt{-1} \) and \( \omega = e^{2\pi i/N_t^k} \)) be the discrete Fourier matrix and

\[
\Gamma_\alpha = \begin{bmatrix}
\frac{1}{\sqrt{N_t}}, & \frac{\alpha^{1/N_t}}{\sqrt{N_t}}, & \cdots, & \frac{\alpha^{(N_t-1)/N_t}}{\sqrt{N_t}}
\end{bmatrix}.
\]
The $\alpha$-circulant matrices $C(\alpha)$ in (2.3) can be simultaneously diagonalized [1, Lemma 2.1] as

$$C(\alpha) = VDV^{-1}, \quad j = 1, 2,$$

where $V = \Gamma_\alpha^{-1} F^*$ and $D = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{N_t})$ with $\lambda_n = -\alpha \frac{2 \pi n}{N_t}$. This implies the block diagonalization of $\mathcal{P}_\alpha$: $\mathcal{P}_\alpha = (V \otimes I_x)(I_x \otimes I_x + D \otimes \mathcal{R}(\Delta tQ)) (V^{-1} \otimes I_x)$. Therefore, the inversion computation of $z := \mathcal{P}_\alpha^{-1} r^k$ can be implemented via 3 steps

Step-(a) $S_1 = (V^{-1} \otimes I_x)r^k$,

Step-(b) $S_{2,n} = (I_x + \lambda_n \mathcal{R}(\Delta tQ))^{-1} S_{1,n}, \quad n = 1, 2, \ldots, N_t$,

Step-(c) $z = (V \otimes I_x)S_2$,

where $S_{j,n} = S_j((n - 1)N_x : nN_x)$ denotes the $n$-th block of $S_j$ for $j = 1, 2$.

By noticing $V^{-1} = F \Gamma_\alpha$ in (2.6), Step-(a) and Step-(c) can be computed efficiently via FFT with $O(N_x N_t \log N_t)$ operations. In Step-(b), we do not have to form the matrix $\mathcal{R}(\Delta tQ)$ in practice. For example, for the trapezoidal rule, i.e., $\mathcal{R}(\Delta tQ) = (I_x + \Delta tQ/2)^{-1}(I_x - \Delta tQ/2)^{-1}$, the linear system in Step-(b) becomes

$$\left((1 + \lambda_n)I_x + (1 - \lambda_n)\frac{\Delta tQ}{2}\right) S_{2,n} = \left(I_x + \frac{\Delta tQ}{2}\right) S_{1,n}. \quad (2.7)$$

How to avoid direct use of $\mathcal{R}(\Delta tQ)$ in Step-(b) heavily depends on the Runge-Kutta method used as the time-integrator. This topic is however beyond the scope of this paper and we will address it in other place.

Here we mainly focus on the convergence properties of (2.4). To this end, we define the stability of the single step method (2.2) in the usual way [20, Chapter IV.3].

**Definition 2.1.** The time-integrator (2.2) is stable if $\max_{z \in \sigma(\Delta tQ)} |\mathcal{R}(z)| \leq 1$, where $\sigma(\Delta tQ)$ denotes the spectrum of $\Delta tQ$.

The next theorem indicates that the stability of time integrator (2.2) implies the convergence of iteration (2.4).

**Theorem 2.2.** Assume that the space discretization matrix $A$ is diagonalizable as $A = V_A D_A V_A^{-1}$. Let $W = I_t \otimes P$ with $P$ being the eigenvector matrix of $Q$, i.e.,

$$P = \begin{bmatrix} V_A \\ V_A \end{bmatrix} \begin{bmatrix} \frac{iD_A^+}{I_x} & -\frac{iD_A^-}{I_x} \\ I_x & I_x \end{bmatrix}. \quad (2.8)$$

Let $err^k = w^k - w$ be the error at the $k$-th iteration of (2.4). Then, for any $k \geq 1$ it holds

$$\|err^{k+1}\|_{W,2} \leq \frac{\alpha}{1 - \alpha} \|err^k\|_{W,2}, \quad \alpha \in (0, 1), \quad (2.9)$$

provided the time-integrator (2.2) is stable.

**Proof.** It is clear that the error $err^k$ satisfies

$$err^{k+1} = err^k - (P_\alpha^{-1} K)err^k, \quad k = 0, 1, \ldots.$$

We have

$$(I_t \otimes P)(P_\alpha^{-1} K)(I_t \otimes P^{-1}) = \text{blkdiag}(P_\alpha^{-1}(z_1)K(z_1), P_\alpha^{-1}(z_2)K(z_2), \ldots, P_\alpha^{-1}(z_{N_x})K(z_{N_x})), \quad (2.10)$$

where $z_j \in \sigma(\Delta tQ)$ is the $j$-th eigenvalue of $\Delta tQ$ and

$$K(z) = I_t + \mathcal{R}(z)B, \quad P_\alpha(z) = I_t + \mathcal{R}(z)C(\alpha). \quad (2.11)$$
Let \( \zeta^k = ((\xi_1^k)^T, (\xi_2^k)^T, \ldots, (\xi_{N_n}^k)^T)^T = (I_t \otimes P)\text{err}^k \). Let \( z \) be an arbitrary eigenvalue of \( \Delta tQ \) with \( \xi^k \in \mathbb{R}^{N_1} \) being the corresponding subvector of \( \zeta^k \). Then, it is clear that
\[
\xi^{k+1} = \xi^k - (P_{\alpha}^{-1}(z)K(z))\xi^k, \quad k = 0, 1, \ldots
\]  
(2.10)

Next we shall verify that (2.10) is equivalent to the following system
\[
\begin{cases}
\xi_{n+1}^{k+1} = R(z)\xi_n^{k+1}, & n = 0, 2, \ldots, N_t - 1, \\
\xi_0^{k+1} = \alpha(\xi_{N_t}^{k+1} - \xi_{N_N}^k), 
\end{cases}
\]  
(2.11)

where \( \xi_{N_t}^k \neq 0 \) for \( k = 0 \) (otherwise for all \( k \geq 1 \) the iterates are zero), and \( \xi^k = (\xi_1^k, \xi_2^k, \ldots, \xi_{N_N}^k)^T \).

Indeed, the matrix-vector form of (2.11) is
\[
(I_t + R(z)C(\alpha))\xi^{k+1} + \alpha \begin{bmatrix} R(z)\xi_N^k \\ 0 \\ \vdots \\ 0 \end{bmatrix} = 0,
\]  
(2.12)

where \( C(\alpha) \) is the matrix given by (2.3). By noticing
\[
\alpha \begin{bmatrix} R(z)\xi_N^k \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} \alpha R(z) \\ \vdots \end{bmatrix} \xi^k = [R(z)B - R(z)C(\alpha)]\xi^k = [(I_t + R(z)B) - (I_t + R(z)C(\alpha))]\xi^k,
\]
we can represent (2.12) as \( P_{\alpha}(z)\xi^{k+1} + (K(z) - P_{\alpha}(z))\xi^k = 0 \), which is exactly (2.10).

Under the assumption that the time-integrator is stable, i.e., \( |R(z)| \leq 1 \), from the first equation in (2.11) we have \( |\xi_{n+1}^{k+1}| = |R(z)||\xi_n^{k+1}| \leq |\xi_n^{k+1}| \), which holds for all \( k \geq 0 \). Hence, from the second equation in (2.11) it holds for any \( k \geq 1 \) that
\[
|\xi_{n+1}^{k+1}| = \alpha |\xi_{n+1}^{k+1} - \xi_{N_N}^k| \leq \alpha |\xi_{n+1}^{k+1}| + \alpha |\xi_{N_N}^k| \leq \alpha |\xi_{n+1}^{k+1}| + \alpha |\xi_{n+1}^k|,
\]
where \( n = 0, 1, \ldots, N_t \). That is, \( |\xi_{n+1}^{k+1}| \leq \frac{\alpha}{1 - \alpha} |\xi_{n+1}^k| \). To summarize, it holds
\[
||\xi^{k+1}||_2 \leq \frac{\alpha}{1 - \alpha} ||\xi^k||_2.
\]  
(2.13)

For \( \zeta^k = ((\xi_1^k)^T, (\xi_2^k)^T, \ldots, (\xi_{N_N}^k)^T)^T \) with any index \( k \), it is clear that
\[
||\zeta^k||_2 = \sqrt{\sum_{j=1}^{2N_n} ||\xi_j^k||_2^2}
\]
Since \( \zeta^k \) is an arbitrary subvector of \( \zeta^k \), it follows from (2.13) that \( ||\zeta^{k+1}||_2 \leq \frac{\alpha}{1 - \alpha} ||\zeta^k||_2 \). This, together with \( \zeta^k = (I_t \otimes P)\text{err}^k \), gives the desired result (2.8).

**Remark 2.1.** It would be interesting to study how the norm of the matrix \( W \) in Theorem 2.2 depends on the mesh size \( \Delta x \). A moderate norm \( ||W||_2 \) as \( \Delta x \to 0 \) is desired since in this case the inequality (2.8) can better reflect the contraction relationship between \( \text{err}^{k+1} \) and \( \text{err}^k \). Since \( A \) is a discrete matrix of the negative Laplacian, i.e., \( A \approx -\Delta \), without loss of generality we assume that the eigenvector matrix \( V_A \) of \( A \) is a unitary matrix (i.e., \( ||V_A||_2 = 1 \)). Hence,
\[
||W||_2 = ||P||_2 = \left\| \begin{bmatrix} V_A & V_A \end{bmatrix} \begin{bmatrix} \frac{1}{2} D_{A}^{\frac{1}{2}} & -iD_{A}^{\frac{1}{2}} \\ I_x & I_x \end{bmatrix} \right\|_2 \leq \left\| \begin{bmatrix} \frac{1}{2} D_{A}^{\frac{1}{2}} & -iD_{A}^{\frac{1}{2}} \\ I_x & I_x \end{bmatrix} \right\|_2.
\]  
(2.14)
Since $D_A$ is the eigenvalue matrix of $A$, it holds $D_A = \Delta x^{-2} \tilde{D}_A$, where $\tilde{D}_A$ is a diagonal matrix satisfying $\|\tilde{D}_A\|_2 \leq C$ with some constant $C$ as $\Delta x \to 0$. Hence,

$$
\left\| \begin{bmatrix} iD_A^{-\frac{1}{2}} & -iD_A^{-\frac{1}{2}} \\ I_x & I_x \end{bmatrix} \right\|_2 \to \left\| \begin{bmatrix} 0 & 0 \\ I_x & I_x \end{bmatrix} \right\|_2 = \sqrt{2}, \text{ as } \Delta x \to 0.
$$

Substituting this into (2.14) gives $\|W\|_2 \leq \sqrt{2}$ as $\Delta x \to 0$.

3. Parameterized two-step time-integrators. Reducing a second-order differential equation to a first-order system as we did in Section 2 actually doubles the storage complexity at each time level. This will be a problem in the high-dimensional cases using very fine space mesh sizes. Due to the second-order temporal derivative, it is more natural to use two-step time-integrators for time discretization. In this section, we consider two classes of representative two-step time-integrators: a parametrized Numerov method and a parametrized two-stage method, both of which are widely used for the second-order differential equations.

3.1. The parameterized Numerov method. The following two-step method is a byproduct of the accuracy analysis of linear multistep methods for second-order differential equations by Dahlquist in 1978 [5]:

$$
U_{n+1} - 2U_n + U_{n-1} \over \Delta t^2 + A(\gamma U_{n+1} + (1-2\gamma)U_n + \gamma U_{n-1}) = \bar{F}_n,
$$

where $\bar{F}_n = \gamma F_{n+2} + (1-2\gamma)F_{n+1} + (1-2\gamma)F_{n-1}$ and $\gamma$ is a free parameter. According to [5], it holds

$$
U_n - U(t_n) = c_2 \Delta t^2 + O(\Delta t^4), \quad c_2 = \frac{1}{12} - \gamma,
$$

where $U(t_n)$ denotes the exact solution of the second-order differential equation (1.2) at $t = t_n$. The parameter $\gamma = \frac{1}{2}$ corresponds to the implicit leap-frog method studied in [24]. The choice $\gamma = \frac{1}{4}$ corresponds to the trapezoidal rule applied to the order reduced system (2.1). (By eliminating the intermediate variables $\{V_n\}$ there, we will obtain a two-step difference equation between $U_{n+1}$, $U_n$ and $U_{n-1}$, just as (3.1) with $\gamma = \frac{1}{4}$.) Finally, we see that the choice $\gamma = \frac{1}{12}$ reverts (3.1) to the classical Numerov method (1.6), for which the discretization error constant $c_2$ varnishes and thus the method is of order 4.

For (3.1), the all-at-once solution via a preconditioned iteration is

$$
u^{k+1} = \nu^k - \mathcal{P}_\alpha^{-1}(\mathcal{K}\nu^k - \nu), \quad k = 0, 1, \ldots, \tag{3.2a}
$$

where $\nu^k = (\nu_{1}^k)^T, (\nu_{2}^k)^T, \ldots, (\nu_{N}^k)^T$. Let $\mathcal{K}\nu = \nu$ and $\nu$ be a suitable term depending on the vectors $\{\bar{F}_n\}$. Here the all-at-once matrix $\mathcal{K}$ and the preconditioner $\mathcal{P}_\alpha$ are

$$
\mathcal{K} = B_1 \otimes I_x + B_2(\gamma) \otimes (\Delta t^2 A), \quad \mathcal{P}_\alpha = C_1(\alpha) \otimes I_x + C_2(\alpha, \gamma) \otimes (\Delta t^2 A),
$$

where the Toeplitz matrices $B_{1,2}$ and the $\alpha$-circulant matrices $C_{1,2}$ are given by (1.7).

**Theorem 3.1.** Suppose that he parameterized Numerov method (3.1) is stable in sense that

$$
\rho(M(z)) \leq 1, \quad \forall z \in \sigma(\Delta t^2 A), \tag{3.3}
$$

where $M(z) := -\begin{bmatrix} 1 + \gamma z & -1 + \frac{2\gamma z}{1 - \gamma} \\ 0 & 1 - \frac{2\gamma z}{1 - \gamma} \end{bmatrix}^{-1} \begin{bmatrix} 1 - \frac{2\gamma z}{1 - \gamma} & 1 + \gamma z \\ -1 - \frac{2\gamma z}{1 - \gamma} & 0 \end{bmatrix}$. Let $\text{err}^k = \nu^k - \nu$ be the error at the $k$-th iteration of (3.2a). Then, with the assumption (3.3) it holds

$$
\|\text{err}^{k+1}\|_{W^2,2} \leq \frac{\alpha}{1-\alpha} \|\text{err}^k\|_{W^2,2}, \quad \alpha \in (0,1), \tag{3.4}
$$
where \( W = \text{blkdiag}(P_1, P_2, \ldots, P_{N_t})(I_t \otimes V_A) \) with \( P_j = (I_t \otimes V_M(z_j))J \) and \( V_A \) being the eigenvector matrix of \( \Delta t^2 A \). Here, \( I_t \in \mathbb{R}^{N_t \times N_t}, I_t \in \mathbb{R}^{(N_t-1) \times (N_t-1)} \) are identity matrices, \( V_M(z_j) \) is the eigenvector matrix of \( M(z_j) \) with \( z_j \) being the \( j \)-th eigenvalue of \( \Delta t^2 A \) and

\[
J = \begin{bmatrix}
J_1 \\
J_2 \\
\vdots \\
J_{N_t-1}
\end{bmatrix}
\quad \text{with} \quad J_n := \begin{bmatrix}
0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\
0 & \cdots & 1 & 0 & \cdots & 0
\end{bmatrix} \in \mathbb{R}^{2 \times N_t},
\tag{3.5}
\]

where the vectors \( \begin{bmatrix} 0 \\ 1 \end{bmatrix} \) and \( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) appear as the \( n \)-th and \((n+1)\)-th column of \( J_n \), respectively.

**Proof.** Let \( z \geq 0 \) be an arbitrary eigenvalue of \( \Delta t^2 A \), i.e., \( z \in \sigma(\Delta t^2 A) \). Then, the parameterized Numerov method (3.1) is

\[
u_{n+1} - 2u_n + u_{n-1} + z(\gamma u_{n+1} + (1 - 2\gamma)u_n + \gamma u_{n-1}) = \Delta t^2 \bar{f}_n,
\tag{3.6}
\]

where \( u_n \) is the component of \( U_n \) corresponding to the eigenvalue \( z \) (similar explanation goes to \( \bar{f}_n \)). To study the stability of (3.6), we equivalently reformulate it as an one-step difference equation

\[
\begin{bmatrix}
u_{n+1} \\ u_n \end{bmatrix} = M(z) \begin{bmatrix}
u_n \\ u_{n-1} \end{bmatrix} + \begin{bmatrix}
1 + \gamma z & -1 + \frac{1-2\gamma}{2}z \\
0 & 1
\end{bmatrix}^{-1} \begin{bmatrix}
0 \\ \Delta t^2 \bar{f}_n
\end{bmatrix},
\]

and therefore \( \rho(M(z)) \leq 1 \) implies the existence of a bound of \( u_n \) for arbitrarily large \( n \).

Let \( \xi^k = ((\xi^k_1)^T, (\xi^k_2)^T, \ldots, (\xi^k_{N_t})^T)^T = (I_t \otimes V_A)err^k \) and \( z \) be an arbitrary eigenvalue of \( \Delta t^2 A \) with \( \xi^k \in \mathbb{R}^{N_t} \) being the corresponding subvector of \( \xi^k \). Then,

\[
\xi^{k+1} = \xi^k - (P_{\alpha}^{-1}(z)K(z))\xi^k, \quad k = 0, 1, \ldots
\tag{3.7}
\]

where \( P_{\alpha}(z) = C_1(\alpha) + zC_2(\alpha, \gamma) \) and \( K(z) = B_1 + zB_2(\gamma) \).

Let \( \xi^k = (\xi_{N_t}^k, \xi_{N_t-1}^k, \ldots, \xi_{0}^k)^T \). Next we shall show that the iteration (3.7) is equivalent to the time stepping system

\[
\begin{align*}
\xi_{n+1}^{k+1} &- \alpha e_{N_t}^{k+1} + \gamma e_{n+1}^{k+1} + (1 - 2\gamma)\xi_{n+1}^{k+1} + \gamma \xi_{n-1}^{k+1} = 0, \quad n = 1, 2, \ldots, N_t, \\
e_0^{k+1} &- \alpha (e_{N_t}^{k+1} - e_{N_t}^{k}), \\
e_1^{k+1} &- \alpha (e_{N_t+1}^{k+1} - e_{N_t+1}^{k}).
\end{align*}
\tag{3.8}
\]

It is easy to verify that the matrix-vector form of (3.8) is

\[
(C_1(\alpha) + zC_2(\alpha, \gamma))\xi^{k+1} - \alpha
\begin{bmatrix}
(1 + \gamma z)e_{N_t}^{k+1} + ((1 - 2\gamma)z - 2)e_{N_t+1}^{k+1} \\
(1 + \gamma z)e_{N_t}^{k+1} \\
\vdots \\
0
\end{bmatrix}
\begin{bmatrix}
0 \\
\vdots \\
0
\end{bmatrix}
= 0.
\tag{3.9}
\]

By noticing

\[
\alpha
\begin{bmatrix}
(1 + \gamma z)e_{N_t}^{k} + ((1 - 2\gamma)z - 2)e_{N_t+1}^{k} \\
(1 + \gamma z)e_{N_t}^{k+1} \\
\vdots \\
0
\end{bmatrix}
= \begin{bmatrix}
\alpha & -2\alpha \\
\alpha & 0
\end{bmatrix}
+ \begin{bmatrix}
\alpha & 0 \\
0 & \alpha
\end{bmatrix}
\xi^k,
\]

\[
(1 + \gamma z)e_{N_t}^{k+1} + ((1 - 2\gamma)z - 2)e_{N_t+1}^{k+1}
\]

\[
(1 + \gamma z)e_{N_t}^{k+1}
\]
we can represent (3.9) as \( P_{\alpha}(z)\xi^{k+1} - (P_{\alpha}(z) - K(z))\xi^k = 0 \), which is exactly the preconditioned fixed-point iteration (3.7).

Now, by letting \( E_n^k = (e_{n+1}^k, e_n^k)^T \) we can represent (3.8) as

\[
\begin{align*}
E_{n+1}^k &= M(z)E_{n+1}^k, \quad n = 0, 1, \ldots, N_t - 1, \\
E_0^k &= \alpha(E_{N_t}^k - E_{N_t}^k).
\end{align*}
\]

(3.10)

Let \( V_M(z) \) and \( D_M(z) \) be respectively the eigenvector and eigenvalue matrices of \( M(z) \), i.e.,

\[
M(z) = V_M(z)D_M(z)V_M^{-1}(z).
\]

Then, by letting \( \tilde{E}_n^k = V_M(z)E_n^k \) we have from (3.10)

\[
\begin{align*}
\tilde{E}_{n+1}^k &= D_M(z)\tilde{E}_{n+1}^k, \quad n = 0, 1, \ldots, N_t - 1, \\
\tilde{E}_0^k &= \alpha(\tilde{E}_{N_t}^k - \tilde{E}_{N_t}^k).
\end{align*}
\]

Under the assumption \( \rho(M(z)) \leq 1 \), it holds \( \|\tilde{E}_{n+1}^k\|_2 \leq \frac{a}{1-\alpha}\|\tilde{E}_n^k\|_2 (\forall n \geq 0) \). The proof of this inequality is the same as the proof for Theorem 2.2 and the details are omitted.

Therefore, \( \|V_M(z)E_{n+1}^k\|_2 \leq \frac{a}{1-\alpha}\|V_M(z)E_n^k\|_2 \) and

\[
\|((\tilde{I}_t \otimes V_M(z))E_{n+1}^k\|_2 \leq \frac{\alpha}{1-\alpha}\|((\tilde{I}_t \otimes V_M(z))E_n^k\|_2, (3.11)
\]

where \( \tilde{I}_t \in \mathbb{R}^{(N_t-1) \times (N_t-1)} \) is an identity matrix and

\[
E^k = ((E_{2,t}^k)^T, (E_{3,t}^k)^T, \ldots, (E_{N_t,t}^k)^T)^T = (e_2^k, e_3^k, e_4^k, \ldots, e_{N_t-1}^k, e_{N_t}^k) \in \mathbb{R}^{2(N_t-1)}.
\]

We now need to represent \( E^k \) by the vector \( \xi^k = (e_2^k, e_3^k, \ldots, e_{N_t}^k)^T \in \mathbb{R}^{N_t} \). By using the matrix \( J \in \mathbb{R}^{2(N_t-1) \times N_t} \) given by (3.5), it holds \( E^k = J\xi^k \) and substituting this into (3.11) gives

\[
\|((\tilde{I}_t \otimes V_M(z))J\xi_{n+1}^k\|_2 \leq \frac{\alpha}{1-\alpha}\|((\tilde{I}_t \otimes V_M(z))J\xi_n^k\|_2,
\]

For the vector \( \zeta^k = ((\xi_1^k)^T, (\xi_2^k)^T, \ldots, (\xi_{N_t}^k)^T)^T \), each subvector \( \xi_j^k \) corresponds to an eigenvalue \( z_j \) of \( \Delta t^2 A \). Hence, by defining \( P_j = (I_t \otimes V_M(z_j))J \) and \( P = \text{blkdiag}(P_1, P_2, \ldots, P_{N_t}) \), we have

\[
\|P\zeta_{n+1}^k\|_2 \leq \frac{\alpha}{1-\alpha}\|P\zeta_n^k\|_2, (3.12)
\]

which together with \( \zeta_{n+1}^{k+1} = (I_t \otimes V_A)e\text{rr}^{k+1} \) gives the desired result (3.4). \( \square \)

3.2. Parametrized two-stage method. We next consider a parametrized two-stage method, which was first introduced by Chawla in 1983 [3]:

\[
\begin{align*}
\tilde{U}_n &= U_n + \gamma \Delta t^2 A(U_{n+1} - 2U_n + U_{n-1}) + \gamma \Delta t^2 (F_{n+1} - 2F_n + F_{n-1}), \\
\frac{U_{n+1} - 2U_n + U_{n-1}}{\Delta t^2} + A\frac{U_{n+1} + 10U_n + U_{n-1}}{12} &= F_{n+1} + 10F_n + F_{n-1},
\end{align*}
\]

(3.13)

where \( \gamma > 0 \) is a parameter and \( n = 1, 2, \ldots, N_t \). It was proved in [3] that this time-integrator is of order 4 for all \( \gamma > 0 \) and that it is unconditionally stable if \( \gamma \geq 1/120 \). We note that the classical Numerov method (the second stage of (3.13)) is of order 4 as well, but it is conditionally stable.

Substituting \( \tilde{U}_{n+1} \) into the second equation gives

\[
\frac{U_{n+1} - 2U_n + U_{n-1}}{\Delta t^2} + A\frac{U_{n+1} + 10U_n + U_{n-1}}{12} + 10\gamma \Delta t^2 A^2\frac{U_{n+1} - 2U_n + U_{n-1}}{12} = F_{n+1}^A, (3.14)
\]
where $F_n^1 = \frac{F_{n+1} + 10F_n + F_{n-1}}{12} - 10\gamma \Delta t^2 A F_{n+1} - 2F_n + F_{n-1}$. (We never use (3.14) in practice due to the matrix quadratic term $(\Delta t^2 A)^2$ and here it appears to describe the preconditioned all-at-once iteration in the following.) Let

$$B_1 = \begin{bmatrix}
1 & 1 \\
-2 & -1 \\
1 & -2 & 1 \\
\vdots & \vdots & \ddots & \ddots \\
1 & -2 & 1
\end{bmatrix}, \quad B_2 = \frac{1}{12} \begin{bmatrix}
1 & 10 & 1 \\
10 & 1 & 1 \\
1 & 10 & 1
\end{bmatrix},$$

$$C_1(\alpha) = \begin{bmatrix}
1 & \alpha & -2\alpha \\
-2 & 1 & \alpha \\
1 & -2 & 1 \\
\vdots & \vdots & \ddots & \ddots \\
1 & -2 & 1
\end{bmatrix}, \quad C_2(\alpha) = \frac{1}{12} \begin{bmatrix}
1 & \alpha & 10\alpha \\
10 & 1 & \alpha \\
1 & 10 & 1
\end{bmatrix}.$$  

(3.15a)

Then, we can solve (3.14) via the preconditioned iteration

$$u^{k+1} = u^k - P_\alpha^{-1}(Ku^k - b), \quad k = 0, 1, \ldots,$$  

(3.15b)

where $u^k = ((U^k_2)^T, (U^k_3)^T, \ldots, (U^k_{N+1})^T)^T$, $b$ is a suitable vector depending on the source terms $\{F_n^1\}$ and $\mathcal{K} = B_1 \otimes I_x + B_2 \otimes (\Delta t^2 A) + \frac{5\gamma}{6} B_1 \otimes (\Delta t^2 A)^2$,

$$\mathcal{P}_\alpha = C_1(\alpha) \otimes I_x + C_2(\alpha) \otimes (\Delta t^2 A) + \frac{5\gamma}{6} C_1(\alpha) \otimes (\Delta t^2 A)^2.$$  

(3.15c)

**Theorem 3.2.** Suppose that the parameterized two-stage method (3.13) is stable in sense that

$$\rho(M(z)) \leq 1, \quad \forall z \in \sigma(\Delta t^2 A),$$

(3.16)

where

$$M(z) := -\begin{bmatrix}
1 + \frac{5\gamma z^2}{12} & \frac{5\gamma z^2}{6} & -1 + \frac{5\gamma z^2}{12} & \frac{5\gamma z^2}{6} \\
\frac{5\gamma z^2}{6} & 1 & -1 & \frac{5\gamma z^2}{6} \\
-1 & \frac{5\gamma z^2}{6} & 1 + \frac{5\gamma z^2}{12} & \frac{5\gamma z^2}{6} \\
\frac{5\gamma z^2}{6} & \frac{5\gamma z^2}{6} & -1 & 0
\end{bmatrix}^{-1}.$$  

Let $\mathbf{err}^k = u^k - \mathbf{w}$ be the error at the $k$-th iteration of (3.15b). Then, with the assumption (3.16) it holds

$$\|\mathbf{err}^{k+1}\|_{W,2} \leq \frac{\alpha}{1 - \alpha} \|\mathbf{err}^k\|_{W,2}, \quad \alpha \in (0, 1),$$

(3.17)

where $\mathbf{W}$ is the matrix given in Theorem 3.1 with the eigenvector matrix $V_M(z)$ of $M(z)$ being replaced.

**Proof.** Let $z \geq 0$ be an arbitrary eigenvalue of $\Delta t^2 A$, i.e., $z \in \sigma(\Delta t^2 A)$. Then, the parameterized two-stage method (3.14) is

$$\left(1 + \frac{z}{12} + \frac{5\gamma z^2}{6}\right) u_{n+1} + 2 \left(-1 + \frac{5z}{12} - \frac{5\gamma z^2}{6}\right) u_n + \left(1 + \frac{z}{12} + \frac{5\gamma z^2}{6}\right) u_{n-1} = \Delta t^2 f_n^1,$$  

(3.18)

where $u_n$ is the component of $U_n$ corresponding to the eigenvalue $z$. To study the stability of (3.18), we equivalently reformulate it as an one-step difference equation

$$\begin{bmatrix}
u_{n+1} \\ u_n
\end{bmatrix} = M(z) \begin{bmatrix}
u_n \\ u_{n-1}
\end{bmatrix} + \left[1 + \frac{z}{12} + \frac{5\gamma z^2}{6} -1 + \frac{5z}{12} - \frac{5\gamma z^2}{6}\right]^{-1} \begin{bmatrix}0 \\ \Delta t^2 f_n^1
\end{bmatrix}.$$
and from this it is clear that $\rho(M(z)) \leq 1$ implies the existence of a bound of $u_n$ for arbitrarily large $n$.

The proof of (3.17) is twofold. First, by letting $\xi^k = ((\xi_1^k)^T, \ldots, (\xi_N^k)^T)^T = (I_t \otimes V_A)\text{err}^k$ and $z$ be an arbitrary eigenvalue of $\Delta t^2 A$ with $\xi^k \in \mathbb{R}^N$ being the corresponding subvector of $\xi^k$ we have

$$
\xi^{k+1} = \xi^k - (P_\alpha^{-1}(z)K(z))\xi^k, \; k = 0, 1, \ldots
$$

where $P_\alpha(z) = C_1(\alpha) + zC_2(\alpha) + \frac{5\alpha}{6}C_1(\alpha)$ and $K(z) = B_1 + zB_2 + \frac{5\alpha}{6}B_1$.

Let $\xi^k = (e_{\beta_0}^k, e_{\beta_1}^k, \ldots, e_{\beta_N}^k)^T$ and then we can show that the components of $\xi^k$ satisfy a special difference equation with an $\alpha$-parameterized head-tail coupled condition (cf. (3.8)). Second, with the same procedure for proving (3.12) we can show $\|P\xi^{k+1}\|_2 \leq \frac{\alpha}{1-\alpha}\|P\xi^k\|_2$, where $P$ is the same matrix appearing in the proof of Theorem 3.1 with the eigenvector matrix $V_M(z)$ of $M(z)$ being replaced.

**Remark 3.1.** Similar to Remark 2.1, it is useful to study $\|W\|_2$ for small mesh size $\Delta x$. Here, we consider the parameterized Numerov method in Section 3.1 and the parameterized two-stage method in Section 3.2 can be treated similarly. As in Remark 2.1 we assume that the eigenvector matrix $V_A$ of $A \approx -\Delta$ is an unitary matrix. Then, from Theorem 3.1 we have

$$
\|W\|_2 = \|\text{blkdiag}(P_1, P_2, \ldots, P_N)(I_t \otimes V_A)\|_2 \\
\leq \max_{j=1,2,\ldots,N} \|P_j\|_2 \leq \|V_M(z_j)\|_2\|J\|_2,
$$

since $P_j = (\tilde{I}_t \otimes V_M(z_j))J$. The matrix $V_M(z_j)$ is the eigenvector matrix of $M(z_j)$ and is given by

$$
V_M(z) = \begin{bmatrix}
1 + \sqrt{\left(\frac{z}{1+\gamma z} - 4\right)\frac{1}{1+\gamma z}} & 1 - \sqrt{\left(\frac{z}{1+\gamma z} - 4\right)\frac{1}{1+\gamma z}} \\
1 & 1
\end{bmatrix},
$$

where $z_j \geq 0$ is an eigenvalue of $\Delta t^2 A$. Using the triangle inequality it holds

$$
\|V_M(z)\|_2 \leq \left\|[1 \; 1] + \begin{bmatrix}
\sqrt{\left(\frac{z}{1+\gamma z} - 4\right)\frac{1}{1+\gamma z}} & -\sqrt{\left(\frac{z}{1+\gamma z} - 4\right)\frac{1}{1+\gamma z}} \\
0 & 0
\end{bmatrix}\right\|_2 \\
= 2 + \frac{1}{2} \sqrt{\left|\frac{z}{1+\gamma z} - 4\right| + \left(\frac{z}{1+\gamma z}\right)^2}.
$$

For $z \in [0, \infty)$, it holds $z/(1 + z\gamma) \in [0, \gamma^{-1}]$. Thus,

$$
\|V_M(z)\|_2 \leq 2 + \max\left\{\sqrt{2}, |2\gamma^{-2} - 4\gamma^{-1}|\right\}
$$

Moreover, for the constant matrix $J$ (cf. (3.6)) a routine calculation yields $\|J\|_2 = \sqrt{2}$, which is independent of the size of $J$. Substituting these into (3.19) gives

$$
\|W\|_2 \leq 2\sqrt{2} + \frac{\sqrt{2}\max\{\sqrt{2}, |2\gamma^{-2} - 4\gamma^{-1}|\}}{2}.
$$

### 3.3. Avoid the matrix quadratic term $(\Delta t^2 A)^2$.

Both the matrices $K$ and $P_\alpha$ in (3.15c) contains the matrix quadratic term $(\Delta t^2 A)^2$, which will be a serious problem for storage and computation cost in practice, especially for high-dimensional problems. For each iteration of algorithm (3.15b), the major computation cost consists of two parts. The first is to form the residual vector $r^k = K w^k - b$ and the second is to compute $P_\alpha^{-1} r^k$. In the parallel circumstance,
the $N_i$ subvectors of $w^k$ and $b$ are stored in the $N_i$ cores and the computation of $r^k$ is naturally parallel as we explained in Section 2. The computation of $P^{-1}r^k$ is based on the diagonalization procedure and the details are also explained in Section 2 (cf. (2.6)). The crucial point for this procedure is Step-b: 
\[
\left( \lambda_{1,n} I_x + \lambda_{2,n}(\Delta t A) + \frac{5\gamma \lambda_{1,n}}{6}(\Delta t^2 A)^2 \right) S_{2,n} = S_{1,n},
\]  
(3.20) 
where $\{\lambda_{1,n}\}$ and $\{\lambda_{2,n}\}$ are the eigenvalues of the $\alpha$-circulant matrices $C_1(\alpha)$ and $C_2(\alpha)$. If $\lambda_{1,n} = 0$, there is only $\Delta t A$ in (3.20). If $\lambda_{1,n} \neq 0$, (3.20) could be reduced into two linear systems concerning $\Delta t A$ only. This is stated in the following Lemma.

**Lemma 3.3.** For any $c \neq 0$ and $b \in \mathbb{C}$, the solution $p$ of the following problem is also the solution of the quadratic linear equation $(I_x + b(\Delta t^2 A) + c(\Delta t^2 A)^2)x = y$:
\[
\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes I_x + \begin{pmatrix} b - i \\ b - i + i c \\ b - i \end{pmatrix} \otimes (\Delta t^2 A) \begin{pmatrix} x \\ \bar{x} \end{pmatrix} = \begin{pmatrix} y \\ \bar{y} \end{pmatrix},
\]  
(3.21a) 
where $i$ is the imaginary unit. The $2 \times 2$ matrix $W$ can be factorized as $W = V_W D_W V_W^{-1}$, where
\[
D_W = \begin{bmatrix} \frac{b - \sqrt{b^2 - 4c}}{2} \\ \frac{b + \sqrt{b^2 - 4c}}{2} \end{bmatrix}, V_W = \begin{bmatrix} -2 - i(b - \sqrt{b^2 - 4c}) \\ -2 + i(b + \sqrt{b^2 - 4c}) \end{bmatrix}.
\]  
(3.21b) 

**Proof.** From (3.21a), by solving the second equation for the auxiliary variable $\bar{x}$ and then substituting $\bar{x}$ into the first equation we will arrive at the quadratic linear equation $(I_x + b(\Delta t^2 A) + c(\Delta t^2 A)^2)x = y$. The factorization of the matrix $W$ follows by some elementary mathematics and the details should be omitted. $\Box$

Let $b = \lambda_{1,n}$ and $c = \frac{5\gamma}{6}$. Then, according to Lemma 3.3 we can solve quadratic linear system (3.20) via the diagonalization procedure:
\[
\begin{cases}
\begin{pmatrix} x^{(b_1)} \\ \bar{x}^{(b_1)} \end{pmatrix} &= \lambda_{1,n}^{-1}(V_W^{-1} \otimes I_x) \begin{pmatrix} S_{1,n} \\ S_{1,n} \end{pmatrix}, \\
\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes I_x + \begin{pmatrix} b - i(\sqrt{b^2 - 4c}) \\ b + i(\sqrt{b^2 - 4c}) \end{pmatrix} \otimes (\Delta t A) \begin{pmatrix} x^{(b_2)} \\ \bar{x}^{(b_2)} \end{pmatrix} &= \begin{pmatrix} x^{(b_1)} \\ \bar{x}^{(b_1)} \end{pmatrix}, \\
S_{2,n} &= (V_W \otimes I_x) \begin{pmatrix} x^{(b_2)} \\ \bar{x}^{(b_2)} \end{pmatrix},
\end{cases}
\]  
(3.22) 
Step-(b1), Step-(b2), Step-(b3),

where $*$ denotes an auxiliary variable that we do not need to get. We see that the two linear systems in Step-(b2) can be solved in parallel and concern $\Delta t^2 A$ only.

Due to the floating point operations it only holds $W \approx V_W D_W V_W^{-1}$ in practice and therefore the roundoff error plays a role for the diagonalization procedure (3.22). According to the analysis in [14], it holds that roundoff error $= O(\epsilon \text{Cond}_2(V_W))$, where $\epsilon$ is the machine precision. The eigenvector matrix $V_W$ changes for every time point index $n$ and in Figure 3.1 we show $\text{Cond}_2(V_W)$ for each time point. We consider two values of $\gamma$: $\gamma = \frac{\lambda}{200}$ (left) and $\gamma = 1$ (right). For $\gamma = 1$ the two-stage method (3.13) is unconditionally stable, while for $\gamma = \frac{\lambda}{200}$ the method is only conditionally stable; cf. Remark 3.3 below for discussion. We see that in all cases tested here it holds $\text{Cond}_2(V_W) = O(10^1)$ and the condition number seems insensitive to $N_i$ and other parameters. Such a moderate condition number only brings negligible roundoff error in practice.
For the two-stage method (3.13) with two values of the parameter \( \gamma \), the condition number of the eigenvector matrix \( V \) in (3.21b) at each time point. Here, \( \alpha = 0.01 \) and \( T = 4 \).

The analysis in the above two subsections reveals that stability of the time-integrator, i.e., \( \rho(M(z)) \leq 1 \), implies robust convergence of the preconditioned fixed-point iteration. Here, we shall study under what condition on \( \gamma \) such a stability holds.

**Remark 3.2 (Stability condition of the parameterized Numerov method).** Let \( z_{\text{max}} > 0 \) be the maximal eigenvalue of \( \Delta t^2 A \). We shall show that the parameterized Numerov method (3.1) is stable if and only if

\[
\gamma + \frac{1}{z_{\text{max}}} \geq \frac{1}{4}. \tag{3.23}
\]

Let \( z \in [0, z_{\text{max}}] \) be an arbitrary eigenvalue of \( \Delta t^2 A \). Then, from Theorem 3.1 we know that the method is stable if \( \rho(M(z)) \leq 1 \) with

\[
M(z) = \begin{bmatrix}
1 + \gamma z & -1 + \frac{1-2\gamma}{2} z & 1 + \gamma z \\
0 & -1 & 0 \\
-1 & 1 & -1
\end{bmatrix}^{-1}.
\]

Let \( \theta = \frac{z}{1+\gamma z} \). Then, it holds \( \lambda(M(z)) = \frac{2-\theta+\sqrt{\theta(4-\theta)}}{2} \). This implies that \( \rho(M(z)) \leq 1 \) if and only if \( \theta \leq 4 \), since otherwise \( \rho(M(z)) = \frac{\sqrt{\theta(\theta-4)+\theta-2}}{2} > 1 \). Since \( \theta \) is an increasing function of \( z \) and thus \( \theta \leq 4 \) for all \( z \in [0, z_{\text{max}}] \) is equivalent to \( \frac{z_{\text{max}}}{1+\gamma z_{\text{max}}} \leq 4 \), i.e., (3.23).

Now, we can use (3.23) to explain the convergence behavior observed in Figure 1.1 (right) for the preconditioned iteration (1.6). For a 2D wave equation defined on a unit domain \( \Omega = (0,1)^2 \) with Dirichlet boundary condition it holds \( z_{\text{max}} = 4(\Delta x)^2(1-\cos((1-\Delta x)\pi)) \) and therefore

\[
z_{\text{max}} = \begin{cases}
7.9877, & (\Delta x, \Delta t) = (\frac{1}{40}, \frac{1}{40}) \\
5.1121, & (\Delta x, \Delta t) = (\frac{1}{40}, \frac{1}{50})
\end{cases}
\]

The classical Numerov method corresponds to \( \gamma = \frac{1}{12} \) and it is clear that \( z_{\text{max}} = 7.9877 \) does not let (3.23) hold, which explains why the residuals grow in Figure 1.1 on the right for \( (\Delta x, \Delta t) = (\frac{1}{40}, \frac{1}{40}) \). On the contrary, for \( (\Delta x, \Delta t) = (\frac{1}{40}, \frac{1}{50}) \) it holds that \( \gamma + \frac{1}{z_{\text{max}}} = \frac{1}{12} + \frac{1}{5.1121} = 0.2789 > \frac{1}{4} \) and thus the Numerov method is stable in this case, which explains why the residuals decay rapidly.

**Remark 3.3 (Stability condition of the parameterized two-stage method (3.13)).** Let \( z_{\text{max}} > 0 \) be the maximal eigenvalue of \( \Delta t^2 A \). We shall show that the two-stage method (3.13)
is stable if and only if

\[
\begin{align*}
\gamma & \geq \frac{z_{\text{max}} - 6}{5z_{\text{max}}} & \text{if } z_{\text{max}} \leq 12, \\
\gamma & \geq \frac{1}{120}, & \text{if } z_{\text{max}} > 12,
\end{align*}
\]

(3.24)

where \( z_{\text{max}} > 0 \) be the maximal eigenvalue of \( \Delta t^2 A \). For the two-stage method (3.13), the concerned matrix \( M(z) \) given in Theorem 3.2 is

\[
M(z) = \begin{bmatrix}
2 - \frac{z}{1 + \frac{5\gamma z}{6}} & -1 \\
1 & 0
\end{bmatrix}.
\]

By letting \( \theta = \frac{z}{1 + \frac{5\gamma z}{6}} \) it is clear that the two eigenvalues of \( M(z) \) in this case is still given by \( \lambda(M(z)) = \frac{2 - \theta + i\sqrt{\theta(4 - \theta)}}{2} \). Hence, \( \theta \leq 4 \) for all \( z \in [0, z_{\text{max}}] \) implies stability of the two-stage hybrid method (3.13). We have

\[
\frac{d\theta}{dz} = \frac{1 - \frac{5\gamma z^2}{6}}{(1 + \frac{5\gamma z}{6})^2},
\]

and from this the maximum of \( \theta \), denoted by \( \theta_{\text{max}} \), is attained at \( z = z_{\text{max}} \) if \( \frac{5\gamma z^2}{6} \leq 1 \); otherwise, \( \theta_{\text{max}} \) is attained at \( z = \sqrt{\frac{6}{5\gamma \theta}} \). For the former case, \( \theta_{\text{max}} \leq 4 \) requires \( \gamma \geq \max \left\{ \frac{6}{5z_{\text{max}}}, \frac{1}{120} \right\} \). Hence, the stability condition for (3.13) is

\[
\gamma \in \left[ \frac{z_{\text{max}} - 6}{5z_{\text{max}}}, \frac{6}{5z_{\text{max}}} \right] \cup \left[ \max \left\{ \frac{6}{5z_{\text{max}}}, \frac{1}{120} \right\}, \infty \right).
\]

It is clear that this is equivalent to (3.24).

4. Conclusion. In this paper, we studied a parallel-in-time algorithms based on diagonalization technique for evolutional problems. We first formulated the space-time discretization into an all-at-once system \( Ku = b \). Then we constructed a block \( \alpha \)-circulant preconditioner \( P_\alpha \) (where \( \alpha \in (0,1) \) is a free parameter), and solve \( Ku = b \) via the following preconditioned iteration scheme

\[
u^{k+1} = u^k - P_\alpha^{-1}(Ku^k - b).
\]

The property of the \( \alpha \)-circulant matrices allowed us to make a block Fourier diagonalization for \( P_\alpha \) and therefore one can compute \( P_\alpha^{-1}(Ku^k - b) \) in highly parallel for all time levels.

We developed a systematic framework to analyze the convergence of the preconditioned iteration by directly studying the error of the algorithm and using the stability of the time stepping scheme. Our analysis includes all one-step time-integrators and two exemplary classes of two-step time-integrators: the parameterized Numerov methods and the parameterized two-stage hybrid methods. We showed that the preconditioned iteration converges linearly with the convergence factor \( \frac{1}{\lambda_{\text{max}}} \), provided that the time-integrator is stable. Our studied significantly generalize the results in many existing works [17,18,18,23,26–28,34], where considerable efforts were devoted to exploring the spectral radius of the preconditioned matrix and this leads to many case-by-case studies depending on the used time-integrator. Even though we focused on wave equations in this paper, the proposed argument is directly applicable to other evolution problems.
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