No. 641 April 2021

# Fourier analysis of a time-simultaneous two-grid algorithm for the one-dimensional heat equation

C. Lohmann, J. Dünnebacke, S. Turek

ISSN: 2190-1767

# Fourier analysis of a time-simultaneous two-grid algorithm for the one-dimensional heat equation

Christoph Lohmann*, Jonas Dünnebacke*, Stefan Turek*

April 8, 2021

**Abstract**

In this work, the convergence behavior of a time-simultaneous two-grid algorithm for the one-dimensional heat equation is studied using Fourier arguments in space. The underlying linear system of equations is obtained by a finite element or finite difference approximation in space while the semi-discrete problem is discretized in time using the $\theta$-scheme. The simultaneous treatment of all time instances leads to a global system of linear equations which provides the potential for a higher degree of parallelization of multigrid solvers due to the increased number of degrees of freedom per spatial unknown.

It is shown that the all-at-once system based on an equidistant discretization in space and time stays well conditioned even if the number of blocked time-steps grows arbitrarily. Furthermore, mesh-independent convergence rates of the considered two-grid algorithm are proved by adopting classical Fourier arguments in space without assuming periodic boundary conditions. The rate of convergence with respect to the Euclidean norm does not deteriorate arbitrarily if the number of blocked time steps increases and, hence, underlines the potential of the solution algorithm under investigation. Numerical studies demonstrate why minimizing the spectral norm of the iteration matrix may be practically more relevant than improving the asymptotic rate of convergence.

2010 *Mathematics Subject Classification*: 65M55; 65M06; 65M60

**Keywords.** Time-simultaneous two-grid; multigrid waveform relaxation; Fourier analysis; heat equation; spectral norm

## 1 Introduction

In the numerical solution of unsteady partial differential equations, time stepping techniques are traditionally used to discretize the continuous problem in time by means of a sequence of spatial subproblems. These have to be solved one after the other due to their dependence on the solution of the previous time level. This inherently sequential process prevents the possibility of simultaneously computing the solution in different time instances and allows only spatial concurrency. While this possibility of parallelization might be sufficient to significantly improve the performance of the simulation when the overall time horizon is small and the spatial domain is highly resolved, further parallelization capabilities are desirable when the solution is sought at many time steps.

For this purpose, various parallel-in-time methods have been developed in the last decades, where the solution at all (or at least several) considered time steps are (iteratively) computed at once. Typical representatives of this class are given by the parareal algorithm [LMT01], PFASST [Min10; EM12], MGRIT [Fal+17a; Fal+17b; Hes+20], space-time multigrid techniques [Hac85; HV95; GN16], and waveform relaxation

*Institute of Applied Mathematics (LS III), TU Dortmund University, Vogelpothsweg 87, D-44227 Dortmund, Germany

[LRS82; GS98; GK02; HVW95] – to name just a few. Further variants and modifications of parallel-in-time methods can be found, e.g., in the review articles by Gander [Gan15] or Ong and Schroder [OS20].

The solution technique analyzed in this work provides an improved performance by blocking several time steps of the fully discretized problem and applying a geometric multigrid solver to the resulting all-at-once system of equations – interpreted as a space-only problem for vector-valued unknowns. This approach is highly related to the parabolic multigrid method introduced in [Hac85] and the multigrid waveform relaxation method developed by Lubich and Ostermann [LO87], in which discrete time integration is performed after applying a geometric multigrid technique to the spatially discretized problem. Dünnebacke et al. [Dün+19] and Dünnebacke et al. [Dün+21] shed additional light on this 'simultaneous-in-time' methodology by reinterpreting the approach to make use of more complex smoothing strategies. Furthermore, the authors focused on practical aspects like the reduced solution time on modern high performance computing (HPC) facilities and possible extensions to nonlinear problems.

The convergence behavior of this, or slightly modified, solution strategies has already been analyzed in several publications. For instance, in [LO87; JV96], the authors proved that the spectral radius of the two-grid iteration matrix does not depend on the number of blocked time steps and, consequently, a uniform asymptotic rate of convergence can to be expected. On the other hand, local Fourier analysis as introduced by Brandt [Bra76] was exploited in [VH95; HV95] to investigate the associated spectral norm, at least for the one-dimensional heat equation. However, the latter results exploit some simplifications by assuming periodic boundary conditions and, hence, just estimate the exact value when Dirichlet boundary data are prescribed. To the best knowledge of the authors, no theoretical results regarding strict and explicitly determined bounds of the spectral norm have been published so far.

Therefore, the present work tries to fill this gap by considering the one-dimensional heat equation using an equidistant discretization in space by finite elements or finite differences and in time by the $\theta$-scheme. The analysis presented below guarantees that the solver converges monotonically with respect to the Euclidean norm even in case of a single (block-)Jacobi smoothing step if an appropriate relaxation parameter is used. For this purpose, a tensor product approach is employed separating spatial and temporal contributions as exploited, e.g., in [Reu02; BH01]. By doing so, Fourier arguments can be used in space while tailor-made bounds are constructed for the resulting temporal subproblems.

This work is organized as follows: In Section 2, foundations of the 'simultaneous-in-time' approach are laid by describing the fully discretized counterpart of the one-dimensional heat equation and summarizing some important properties. Section 3 introduces general results which will be exploited frequently throughout this work. Section 4 is concerned with the derivation of a bound for the condition number, which guarantees well-conditioned all-at-once problems no matter how many time steps are blocked. In Section 5, several properties of the (block-)Jacobi method/smoother are established while, eventually, the two-grid solver is introduced and its convergence is analyzed in Section 6.

# 2 Global space-time discretization

In this work, we focus on the one-dimensional heat equation

$$\frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) = s(x,t) \quad \text{in } \Omega \times (0,T), \tag{1a}$$

$$u(x,t) = u_{\mathrm{D}} \quad \text{on } \partial\Omega \times (0,T), \tag{1b}$$

$$u(x,0) = u_0(x) \quad \text{on } \Omega, \tag{1c}$$

where $\Omega = (0,1)$ is the unit interval and $T > 0$ denotes the final time. Furthermore, the initial data and external source function are given by $u_0 : \Omega \to \mathbb{R}$ and $s : \Omega \times (0,T) \to \mathbb{R}$, respectively, while $u_{\mathrm{D}} : \partial\Omega \to \mathbb{R}$ denotes the prescribed Dirichlet boundary data. For the sake of simplicity, we restrict our attention to the case of homogeneous boundary conditions and vanishing source terms, i.e., $u_{\mathrm{D}} = 0$ and $s = 0$, but notice that the general case can be treated similarly.

The partial differential equation is discretized in space either by finite differences (FD) or in terms of linear finite elements (FE) using $N \in \mathbb{N}$ equidistantly distributed nodes located in the interior of the domain $\Omega$, i.e., $x_i \coloneqq i(N+1)^{-1}$, $i = 1, \dots, N$. Then the time-dependent vector of degrees of freedom $\mathrm{u}(t) = \big(u_1(t), \dots, u_N(t)\big)^\top : [0,T] \to \mathbb{R}^N$ (approximating the solution $u(x,t)$ in $x_1, \dots, x_N$) solves the semi-discrete counterpart of (1)

$$\mathrm{M}\frac{\mathrm{du}(t)}{\mathrm{d}t} + \mathrm{Du}(t) = 0 \quad \text{in } (0,T), \tag{2a}$$

$$\mathrm{u}(0) = \mathrm{u}^{(0)} \coloneqq \big(u_0(\mathbf{x}_1), \dots, u_0(\mathbf{x}_N)\big)^\top, \tag{2b}$$

where $\mathrm{M} \in \mathbb{R}^{N\times N}$ and $\mathrm{D} \in \mathbb{R}^{N\times N}$ denote the mass matrix and the discrete counterpart of the negative laplacian, respectively. Obviously, both matrices depend on the underlying discretization technique: While in the context of linear finite elements, the matrices coincide with

$$\mathrm{M}_{\mathrm{FE}} = \frac{1}{6}(N+1)^{-1}\begin{pmatrix} 4 & 1 & & \\ 1 & 4 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 4 \end{pmatrix}, \quad \mathrm{D}_{\mathrm{FE}} = (N+1)\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}$$

the well-known central difference approximation of the second derivative leads to

$$\mathrm{M}_{\mathrm{FD}} = \mathrm{I} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}, \quad \mathrm{D}_{\mathrm{FD}} = (N+1)^2\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} \tag{3}$$

for finite differences. The theoretical investigations presented below highly exploit the fact that all four matrices have constant diagonal entries, hereafter denoted by $m_{ii}$ and $d_{ii}$, and possess a common set of orthonormal eigenvectors $(\mathrm{w}^{(\ell)})_{\ell=1,\dots,N}$. These vectors can be written as (cf. [Hac13, Section 2.4])

$$\mathrm{w}^{(\ell)} = \sqrt{2(N+1)^{-1}}\Big(\sin\big(\pi k\ell(N+1)^{-1}\big)\Big)_{k=1}^{N}, \quad \ell = 1, \dots, N$$

while the associated eigenvalues are given by [Hac13, Section 2.4]

$$m^{(\ell)} = 1, \quad d^{(\ell)} = 2d_{ii}\sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) = 2d_{ii}s_\ell^2, \quad \ell = 1, \dots, N \tag{4}$$

for finite differences and

$$m^{(\ell)} = m_{ii}\Big(\tfrac{1}{2} + \cos^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\Big) = m_{ii}\Big(\tfrac{3}{2} - \sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\Big) = m_{ii}\big(\tfrac{3}{2} - s_\ell^2\big), \quad \ell = 1, \dots, N, \tag{5a}$$

$$d^{(\ell)} = 2(N+1)\big(1 - \cos(\pi\ell(N+1)^{-1})\big) = 2d_{ii}\sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) = 2d_{ii}s_\ell^2, \quad \ell = 1, \dots, N \tag{5b}$$

otherwise, where we used the abbreviations

$$s_\ell \coloneqq \sin\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big), \quad c_\ell \coloneqq \cos\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big), \qquad \ell = 1, \dots, N \tag{6}$$

to simplify notation. Note that in both cases the eigenvalues of D are sorted in a strictly increasing manner, i.e., $d^{(1)} < d^{(2)} < \ldots < d^{(N)}$, and only differ by the scaling parameter $h = (N+1)^{-1}$. On the other hand, the eigenvalues of the mass matrix satisfy $m^{(1)} \geqslant m^{(2)} \geqslant \ldots \geqslant m^{(N)}$, which is trivially satisfied for finite differences due to the fact that $m^{(\ell)} = 1$ for all $\ell = 1, \dots, N$. Furthermore, it is easy to verify that the following inequalities are valid:

$$0 < d^{(\ell)} < 2d_{ii}, \qquad \ell = 1, \dots, N, \tag{7}$$

$$\zeta m_{ii} \leqslant m^{(\ell)} \leqslant (2-\zeta)m_{ii}, \quad \ell = 1, \dots, N \tag{8}$$

Here, the quantity $\zeta$ is used to combine inequalities for both discretizations using the values

$$\zeta = 1 \quad \text{for finite differences,} \qquad \zeta = \tfrac{1}{2} \quad \text{for finite elements.}$$

In what follows, we omit the subscripts 'FE' and 'FD' for the sake of clarity and, whenever necessary, distinguish between both spatial discretizations by exploiting $\zeta \in \{\frac{1}{2}, 1\}$.

It is worth mentioning that the linear finite element discretization based on the lumped mass matrix $\tilde{\mathrm{M}}_{\mathrm{FE}} = (N+1)^{-1}\mathrm{I}$ provides the same semi-discrete problem as for finite differences, except for a different scaling. Indeed, we have $\tilde{\mathrm{M}}_{\mathrm{FE}} = (N+1)^{-1}\mathrm{M}_{\mathrm{FD}}$ and $\mathrm{D}_{\mathrm{FE}} = (N+1)^{-1}\mathrm{D}_{\mathrm{FD}}$. Therefore, the below results for finite differences readily hold for a finite element discretization using the lumped mass matrix, too, and this special treatment does not have to be considered separately.

After discretization of the heat equation in space using finite differences or finite elements, application of the two-level $\theta$-scheme, $\theta \in [0,1]$, to the system of ordinary differential equations (2) leads to the fully discretized problem

$$\mathrm{A}\mathrm{u}^{(n+1)} + \mathrm{B}\mathrm{u}^{(n)} = 0, \quad n = 0, \dots, K-1, \tag{9a}$$

$$\mathrm{A} \coloneqq \mathrm{M} + \theta\tau\mathrm{D}, \quad \mathrm{B} \coloneqq -\mathrm{M} + (1-\theta)\tau\mathrm{D}, \tag{9b}$$

where the *constant* time increment $\tau > 0$ is chosen so that $K\tau = T$ for some number of time steps $K \in \mathbb{N}$. Therefore, the discrete vector of degrees of freedom $\mathrm{u}^{(n)} \in \mathbb{R}^N$ approximates the semi-discrete solution $\mathrm{u}(\cdot, t)$ in $t = t_n \coloneqq n\tau$. In what follows, it is assumed that the time step restriction

$$\kappa \coloneqq \zeta m_{ii} - (1-2\theta)\tau d_{ii} \geqslant 0 \tag{10}$$

is valid. This inequality is particularly satisfied for $\theta \geqslant \frac{1}{2}$ or for sufficiently small time increments $\tau$ in the order of $N^{-2}$. Thus, the CFL-like condition (10) is similar to commonly used stability conditions and does not restrict $\tau$ artificially.

In problem (9), the solution $\mathrm{u}^{(n+1)}$ has to be computed sequentially from time step to time step because $\mathrm{u}^{(n+1)}$ depends on $\mathrm{u}^{(n)}$ which again depends on $\mathrm{u}^{(n-1)}$ and so forth. Therefore, frequently used parallelization techniques are only applicable in space which might not be satisfactory if $K \gg N$. To avoid this bottleneck and increase the number of degrees of freedom, we block all time steps and construct a single all-at-once system of equations

$$\mathbf{S}_K\mathbf{u} = \mathbf{b} \quad :\Longleftrightarrow \quad \begin{pmatrix} \mathrm{A} & & & \\ \mathrm{B} & \mathrm{A} & & \\ & \ddots & \ddots & \\ & & \mathrm{B} & \mathrm{A} \end{pmatrix} \begin{pmatrix} \mathrm{u}^{(1)} \\ \mathrm{u}^{(2)} \\ \vdots \\ \mathrm{u}^{(K)} \end{pmatrix} = \begin{pmatrix} -\mathrm{B}\mathrm{u}^{(0)} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{11}$$

for computing the global solution vector $\mathbf{u} = \big((\mathrm{u}^{(1)})^\top, \dots, (\mathrm{u}^{(K)})^\top\big)^\top \in \mathbb{R}^{NK}$, which contains the discrete solution $\mathrm{u}^{(n)}$ at all time steps $n = 1, \dots, K$. Then the global system matrix $\mathbf{S}_K \in \mathbb{R}^{NK \times NK}$ is a block matrix composed of $K \times K$ spatial matrices while the right hand side vector $\mathbf{b} \in \mathbb{R}^{NK}$ depends on given data like the initial condition $\mathrm{u}^{(0)}$ (or non-vanishing source terms $s$ and boundary conditions $u_{\mathrm{D}}$).

In the next section, we show that the condition number of $\mathbf{S}_K$ cannot grow arbitrarily if $K$ increases. Therefore, system (11) stays well conditioned no matter how the number of blocked time steps is chosen. The remainder of this work focuses on an adapted two-grid solver for the above mentioned linear system of equations which uses a (block-)Jacobi method for smoothing purposes as considered in [Dün+21]. We will see that the so defined algorithm possesses a convergence rate which is bounded from above by a constant which possibly depends on the CFL number $\lambda = \tau h^{-2}$, but not on the mesh size $h$, the time increment $\tau$, and the total number of time steps $K$ per se.

The key idea of these theoretical investigations is the fact that the matrices $\alpha\mathrm{M} + \beta\mathrm{D}$ and $(\alpha\mathrm{M} + \beta\mathrm{D})^{-1}$ possess the same eigenvectors $\mathrm{w}^{(1)}, \dots, \mathrm{w}^{(N)}$ as mentioned above for all $\alpha, \beta \in \mathbb{R}$, at least as long as these matrices exist. In addition, the associated eigenvalues are given by $\alpha m^{(\ell)} + \beta d^{(\ell)}$ and $(\alpha m^{(\ell)} + \beta d^{(\ell)})^{-1}$ for all $\ell = 1, \dots, N$, respectively. In particular, the eigenvalues of A and B as defined in (9b) are given by

$$a^{(\ell)} = m^{(\ell)} + \theta\tau d^{(\ell)}, \quad b^{(\ell)} = -m^{(\ell)} + (1-\theta)\tau d^{(\ell)}, \qquad \ell = 1, \dots, N \tag{12}$$

and satisfy

$$a^{(\ell)} - b^{(\ell)} = 2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)} > 0 \tag{13}$$

regardless of the considered spatial discretization because

$$\begin{aligned} 2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)} &\geqslant 2m^{(\ell)} \geqslant 2\zeta m_{ii} > 0 && \text{if } \theta \geqslant \tfrac{1}{2}, \\ 2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)} &> 2\big(\zeta m_{ii} - (1-2\theta)\tau d_{ii}\big) \geqslant 0 && \text{if } \theta < \tfrac{1}{2} \end{aligned}$$

by virtue of (7), (8), and (10).

# 3 Preliminary results

Before the time-simultaneous system of equations and a corresponding two-grid solver are analyzed, we first formulate some general statements which will be exploited frequently in the course of this work.

The first lemma shows that the spectral norm of a $2 \times 2$ block-matrix can be estimated in terms of the spectral norms of all involved submatrices.

**Lemma 1.** *Let $\mathrm{A}_1, \dots, \mathrm{A}_4 \in \mathbb{R}^{M \times M}$, $M \in \mathbb{N}$, and $a_1, \dots, a_4 \geqslant 0$ be upper bounds of the corresponding spectral norm, i.e., $\|\mathrm{A}_i\|_2 \leqslant a_i$ for all $i = 1, \dots, 4$. Then the following inequality holds:*

$$\left\| \begin{pmatrix} \mathrm{A}_1 & \mathrm{A}_2 \\ \mathrm{A}_3 & \mathrm{A}_4 \end{pmatrix} \right\|_2 \leqslant \left\| \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \right\|_2 \tag{14}$$

*Proof.* To prove the statement, let $\mathrm{u}_1, \mathrm{u}_2 \in \mathbb{R}^M$ be arbitrary. We then have

$$\begin{aligned} \left\| \begin{pmatrix} \mathrm{A}_1 & \mathrm{A}_2 \\ \mathrm{A}_3 & \mathrm{A}_4 \end{pmatrix} \begin{pmatrix} \mathrm{u}_1 \\ \mathrm{u}_2 \end{pmatrix} \right\|_2 &= \left\| \begin{pmatrix} \mathrm{A}_1\mathrm{u}_1 + \mathrm{A}_2\mathrm{u}_2 \\ \mathrm{A}_3\mathrm{u}_1 + \mathrm{A}_4\mathrm{u}_2 \end{pmatrix} \right\|_2 = \left\| \begin{pmatrix} \|\mathrm{A}_1\mathrm{u}_1 + \mathrm{A}_2\mathrm{u}_2\|_2 \\ \|\mathrm{A}_3\mathrm{u}_1 + \mathrm{A}_4\mathrm{u}_2\|_2 \end{pmatrix} \right\|_2 \\ &\leqslant \left\| \begin{pmatrix} a_1\|\mathrm{u}_1\|_2 + a_2\|\mathrm{u}_2\|_2 \\ a_3\|\mathrm{u}_1\|_2 + a_4\|\mathrm{u}_2\|_2 \end{pmatrix} \right\|_2 = \left\| \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \begin{pmatrix} \|\mathrm{u}_1\|_2 \\ \|\mathrm{u}_2\|_2 \end{pmatrix} \right\|_2 \\ &\leqslant \left\| \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \right\|_2 \left\| \begin{pmatrix} \|\mathrm{u}_1\|_2 \\ \|\mathrm{u}_2\|_2 \end{pmatrix} \right\|_2 = \left\| \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \right\|_2 \left\| \begin{pmatrix} \mathrm{u}_1 \\ \mathrm{u}_2 \end{pmatrix} \right\|_2, \end{aligned}$$

which proves the statement by definition of the spectral norm. □

The statements summarized in the following lemma will be used to (sharply) estimate the spectral norm, spectral radius, and condition number of global matrices by 'partially diagonalizing' them by means of the set of spatial eigenvectors $\mathrm{w}^{(1)}, \dots, \mathrm{w}^{(N)}$. These results provide the possibility of analyzing the matrix properties separately for each (spatial) Fourier mode.

**Lemma 2.** *Let $\mathbf{A} \in \mathbb{R}^{M \times M}$, $M \in \mathbb{N}$, and $S_1, \dots, S_R \subset \mathbb{R}^M$, $R \in \{1, \dots, M\}$, be orthogonal subspaces satisfying $S_1 + \ldots + S_R = \mathbb{R}^M$ and $\mathbf{A}S_i \subseteq S_i$ for all $i = 1, \dots, R$. Then the following identities are valid:*

$$\|\mathbf{A}\|_2 = \max_{j=1,\dots,R} \|\mathbf{A}\|_{2,S_j} = \max_{j=1,\dots,R} \sqrt{\lambda_{\max,S_j}(\mathbf{A}^\top\mathbf{A})}, \tag{15}$$

$$\operatorname{spr}(\mathbf{A}) = \max_{j=1,\dots,R} \operatorname{spr}_{S_j}(\mathbf{A}), \tag{16}$$

$$\operatorname{cond}_2(\mathbf{A}) = \frac{\max_{j=1,\dots,R} \sqrt{\lambda_{\max,S_j}(\mathbf{A}^\top\mathbf{A})}}{\min_{j=1,\dots,R} \sqrt{\lambda_{\min,S_j}(\mathbf{A}^\top\mathbf{A})}}, \tag{17}$$

*where*

$$\begin{aligned} \|\mathbf{A}\|_{2,S} &:= \max_{\mathbf{v} \in S \setminus \{\mathbf{0}\}} \frac{\|\mathbf{A}\mathbf{v}\|_2}{\|\mathbf{v}\|_2}, && S \subseteq \mathbb{R}^M, \\ \operatorname{spr}_S(\mathbf{A}) &:= \max\big\{|\lambda| \;\big|\; \exists \lambda \in \mathbb{C}, \mathbf{v} \in (S + \imath S) \setminus \{\mathbf{0}\} : \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\big\}, && S \subseteq \mathbb{R}^M, \\ \lambda_{\min,S}(\mathbf{A}) &:= \min\big\{\lambda \in \mathbb{R} \;\big|\; \exists \mathbf{v} \in S \setminus \{\mathbf{0}\} : \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\big\}, && S \subseteq \mathbb{R}^M, \\ \lambda_{\max,S}(\mathbf{A}) &:= \max\big\{\lambda \in \mathbb{R} \;\big|\; \exists \mathbf{v} \in S \setminus \{\mathbf{0}\} : \mathbf{A}\mathbf{v} = \lambda\mathbf{v}\big\}, && S \subseteq \mathbb{R}^M. \end{aligned}$$

*Proof.* • To prove statement (15), let $\mathbf{u} \in \mathbb{R}^M \setminus \{\mathbf{0}\}$ be arbitrary. Then there exist coefficients $\alpha_1, \ldots, \alpha_R \in \mathbb{R}$ and normalized vectors $\mathbf{w}_1 \in S_1, \ldots, \mathbf{w}_R \in S_R$ so that

$$\mathbf{u} = \alpha_1 \mathbf{w}_1 + \ldots + \alpha_R \mathbf{w}_R, \quad \|\mathbf{u}\|_2^2 = \alpha_1^2 + \ldots + \alpha_R^2.$$

Due to the fact that the subspaces $S_1, \ldots, S_R$ are orthogonal to each other and $\mathbf{A}\mathbf{w}_j \in S_j$ for all $j = 1, \ldots, R$, we have $(\mathbf{A}\mathbf{w}_j)^\top(\mathbf{A}\mathbf{w}_k) = 0$ for all $j, k = 1, \ldots, R$, $j \neq k$, and, hence,

$$\begin{aligned}
\|\mathbf{A}\mathbf{u}\|_2^2 = (\mathbf{A}\mathbf{u})^\top(\mathbf{A}\mathbf{u}) &= (\alpha_1 \mathbf{A}\mathbf{w}_1 + \ldots + \alpha_R \mathbf{A}\mathbf{w}_R)^\top(\alpha_1 \mathbf{A}\mathbf{w}_1 + \ldots + \alpha_R \mathbf{A}\mathbf{w}_R) \\
&= \alpha_1^2 \|\mathbf{A}\mathbf{w}_1\|_2^2 + \ldots + \alpha_R^2 \|\mathbf{A}\mathbf{w}_R\|_2^2 \\
&\leqslant \Big( \max_{j=1,\ldots,R} \|\mathbf{A}\mathbf{w}_j\|_2^2 \Big)(\alpha_1^2 + \ldots + \alpha_R^2) \\
&\leqslant \bigg( \max_{j=1,\ldots,R} \Big( \max_{\mathbf{v}_j \in S_j \setminus \{\mathbf{0}\}} \frac{\|\mathbf{A}\mathbf{v}_j\|_2^2}{\|\mathbf{v}_j\|_2^2} \Big) \bigg) \|\mathbf{u}\|_2^2,
\end{aligned}$$

which proves that $\|\mathbf{A}\|_2$ is bounded from above by the right hand side of (15). Equality then follows directly from the fact that there exist $k \in \{1, \ldots, R\}$ and some vector $\mathbf{w} \in S_k \setminus \{\mathbf{0}\}$ so that

$$\max_{j=1,\ldots,R} \Big( \max_{\mathbf{v}_j \in S_j \setminus \{\mathbf{0}\}} \frac{\|\mathbf{A}\mathbf{v}_j\|_2}{\|\mathbf{v}_j\|_2} \Big) = \max_{\mathbf{v}_k \in S_k \setminus \{\mathbf{0}\}} \frac{\|\mathbf{A}\mathbf{v}_k\|_2}{\|\mathbf{v}_k\|_2} = \frac{\|\mathbf{A}\mathbf{w}\|_2}{\|\mathbf{w}\|_2} \leqslant \|\mathbf{A}\|_2. \tag{18}$$

- Statement (17) can be shown similarly.
- To show (16), let $\mathbf{u} \in \mathbb{C}^M$ be a normalized eigenvector of $\mathbf{A}$ associated with the largest absolute eigenvalue $\lambda \in \mathbb{C}$. Then there exist coefficients $\alpha_1, \beta_1, \ldots, \alpha_R, \beta_R \in \mathbb{R}$ and normalized vectors $\mathbf{v}_1, \mathbf{w}_1 \in S_1, \ldots, \mathbf{v}_R, \mathbf{w}_R \in S_R$ so that

$$\mathbf{u} = (\alpha_1 \mathbf{v}_1 + \ldots + \alpha_R \mathbf{v}_R) + \imath(\beta_1 \mathbf{w}_1 + \ldots + \beta_R \mathbf{w}_R), \quad \|\mathbf{u}\|_2^2 = \alpha_1^2 + \beta_1^2 + \ldots + \alpha_R^2 + \beta_R^2 = 1,$$

where $\imath$ denotes the imaginary unit, i.e., $\imath^2 = -1$. Furthermore, there exists some $k \in \{1, \ldots, R\}$ so that $\alpha_k^2 + \beta_k^2 \neq 0$ and

$$\begin{aligned}
\mathbf{v}^\top \lambda(\alpha_k \mathbf{v}_k + \imath\beta_k \mathbf{w}_k) &= \delta_{kj} \mathbf{v}^\top \lambda \mathbf{u} = \delta_{kj} \mathbf{v}^\top \mathbf{A}\mathbf{u} \\
&= \delta_{kj} \mathbf{v}^\top \mathbf{A}(\alpha_j \mathbf{v}_j + \imath\beta_j \mathbf{w}_j) = \mathbf{v}^\top \mathbf{A}(\alpha_k \mathbf{v}_k + \imath\beta_k \mathbf{w}_k), \quad \mathbf{v} \in S_j, \quad j = 1, \ldots, R.
\end{aligned}$$

Therefore, the vector $\alpha_k \mathbf{v}_k + \imath\beta_k \mathbf{w}_k \in S_k + \imath S_k$ is an eigenvector of $\mathbf{A}$ corresponding to the largest absolute eigenvalue $\lambda$ and, hence,

$$\operatorname{spr}(\mathbf{A}) \leqslant \operatorname{spr}_{S_k}(\mathbf{A}) \leqslant \Big( \max_{j=1,\ldots,R} \operatorname{spr}_{S_j}(\mathbf{A}) \Big).$$

The other inequality holds trivially by definition. □

The above lemma provides a possibility of decomposing the analysis of global matrices into some spatial subproblems which can be interpreted as a time-simultaneous discretization of a scalar ordinary differential equation. We will see that the resulting systems of equations have still $K$ unknowns while the corresponding system matrices are of lower bidiagonal Toeplitz form. The spectral norm of these matrices can be analyzed using the following theorem.

**Theorem 3.** *Let* $\mathrm{E}, \mathrm{F} \in \mathbb{R}^{M \times M}$, $M \geqslant 2$, *be given by*

$$\mathrm{E} = \begin{pmatrix} e_1 & & & \\ e_2 & e_1 & & \\ & \ddots & \ddots & \\ & & e_2 & e_1 \end{pmatrix}, \qquad \mathrm{F} = \begin{pmatrix} f_1 & & & \\ f_2 & f_1 & & \\ & \ddots & \ddots & \\ & & f_2 & f_1 \end{pmatrix}, \tag{19}$$

*where* $e_1, e_2, f_1, f_2 \in \mathbb{R}$ *satisfy* $|f_2| < |f_1|$. *Then the spectral norm of* $\mathrm{F}^{-1}\mathrm{E}$ *is bounded from above by*

$$\|\mathrm{F}^{-1}\mathrm{E}\|_2 \leqslant \max\Big(\frac{|e_1 - e_2|}{|f_1 - f_2|}, \frac{|e_1 + e_2|}{|f_1 + f_2|}\Big) = \begin{cases} \frac{|e_1-e_2|}{|f_1-f_2|} & : \eta < 0, \\ \frac{|e_1+e_2|}{|f_1+f_2|} & : \eta \geqslant 0, \end{cases} \tag{20}$$

*where* $\eta = (f_1 e_2 - f_2 e_1)(f_1 e_1 - f_2 e_2)$.

*Proof.* For a detailed proof, the interested reader is referred to the appendix. □

The proposed bound (20) will be used in the following sections to prove the monotone convergence with respect to the Euclidean norm of iterative solvers for the time-simultaneous system (11). Less restrictive estimates exploiting the submultiplicativity $\|\mathrm{F}^{-1}\mathrm{E}\|_2 \leqslant \|\mathrm{F}^{-1}\|_2\|\mathrm{E}\|_2$ do not suffice to show the monotone convergence for some configurations.

While the estimates established in Theorem 3 will suffice to prove the $K$-, $\tau$-, and $h$-independent rate of convergence of the considered two-grid algorithm, they might be inaccurate if $K$ and/or $\tau$ are very small. Then, for instance, the Gershgorin circle theorem [Ger31] or the eigenvalue estimate as proposed in [Tar90] might provide more accurate, possibly parameter-dependent bounds. However, the derivation of such estimates is beyond the scope of this work.

# 4 Condition number of global system matrix

While the global system of equations (11) algebraically possesses the same solution as the sequential counterpart (9), blocking several time steps might result in an ill-conditioned problem. This would make the solution very sensitive to slight perturbations of the system matrix $\mathbf{S}_K$ and/or right hand side vector $\mathbf{b}$. In what follows, we prove that this is actually not the case and the condition number is bounded from above by a value which at least does not depend on $K$.

**Theorem 4.** *The condition number of the system matrix* $\mathbf{S}_K$ *is bounded from above by*

$$\mathrm{cond}_2(\mathbf{S}_K) := \|\mathbf{S}_K\|_2 \|\mathbf{S}_K^{-1}\|_2 \leqslant \frac{\max_{\ell=1,\dots,N}\big(a^{(\ell)} + |b^{(\ell)}|\big)}{\min_{\ell=1,\dots,N}\big(a^{(\ell)} - |b^{(\ell)}|\big)}, \tag{21}$$

*where* $a^{(\ell)}$ *and* $b^{(\ell)}$, $\ell = 1, \dots, N$, *are the eigenvalues of* $\mathrm{A}$ *and* $\mathrm{B}$ *as introduced in* (12).

*Proof.* To begin with, we recall that the matrices A and B posses the same set of eigenvectors $\mathrm{w}^{(1)}, \dots, \mathrm{w}^{(N)}$. Therefore, the global system matrix $\mathbf{S}_K$ satisfies

$$\begin{aligned} \mathbf{S}_K(\mathrm{v} \otimes \mathrm{w}^{(\ell)}) &= \begin{pmatrix} \mathrm{A} & & & \\ \mathrm{B} & \mathrm{A} & & \\ & \ddots & \ddots & \\ & & \mathrm{B} & \mathrm{A} \end{pmatrix} \begin{pmatrix} v_1 \mathrm{w}^{(\ell)} \\ v_2 \mathrm{w}^{(\ell)} \\ \vdots \\ v_K \mathrm{w}^{(\ell)} \end{pmatrix} = \begin{pmatrix} a^{(\ell)}\mathrm{I} & & & \\ b^{(\ell)}\mathrm{I} & a^{(\ell)}\mathrm{I} & & \\ & \ddots & \ddots & \\ & & b^{(\ell)}\mathrm{I} & a^{(\ell)}\mathrm{I} \end{pmatrix} \begin{pmatrix} v_1 \mathrm{w}^{(\ell)} \\ v_2 \mathrm{w}^{(\ell)} \\ \vdots \\ v_K \mathrm{w}^{(\ell)} \end{pmatrix} \\ &= (\mathrm{S}_K^{(\ell)}\mathrm{v}) \otimes \mathrm{w}^{(\ell)}, \quad \mathrm{v} \in \mathbb{R}^K, \quad \ell = 1, \dots, N, \end{aligned} \tag{22}$$

where $\otimes$ denotes the well-known Kronecker product and the auxiliary matrix $\mathrm{S}_K^{(\ell)} \in \mathbb{R}^{K \times K}$ reads

$$\mathrm{S}_K^{(\ell)} = \begin{pmatrix} a^{(\ell)} & & & \\ b^{(\ell)} & a^{(\ell)} & & \\ & \ddots & \ddots & \\ & & b^{(\ell)} & a^{(\ell)} \end{pmatrix}.$$

Thus, the subspaces $S_\ell = \mathbb{R}^K \otimes \mathrm{w}^{(\ell)}$, $\ell = 1, \dots, N$, are invariant under multiplication with $\mathbf{S}_K$, that is, $\mathbf{S}_K S_\ell \subseteq S_\ell$, and, according to Lemma 2, the condition number of $\mathbf{S}_K$ can be expressed by

$$\mathrm{cond}_2(\mathbf{S}_K) = \frac{\max_{\ell=1,\dots,N} \sqrt{\lambda_{\max,S_\ell}(\mathbf{S}_K^\top \mathbf{S}_K)}}{\min_{\ell=1,\dots,N} \sqrt{\lambda_{\min,S_\ell}(\mathbf{S}_K^\top \mathbf{S}_K)}} = \frac{\max_{\ell=1,\dots,N} \sqrt{\lambda_{\max}\big((\mathrm{S}_K^{(\ell)})^\top (\mathrm{S}_K^{(\ell)})\big)}}{\min_{\ell=1,\dots,N} \sqrt{\lambda_{\min}\big((\mathrm{S}_K^{(\ell)})^\top (\mathrm{S}_K^{(\ell)})\big)}}$$

because $(\mathrm{w}^{(\ell)})_{\ell=1,\dots,N}$ is an orthogonal eigenbasis of $\mathbb{R}^N$ and similarly as above

$$\mathbf{S}_K^\top \mathbf{S}_K(\mathrm{v}\otimes \mathrm{w}^{(\ell)}) = \big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\mathrm{v}\big)\otimes \mathrm{w}^{(\ell)} \in (\mathbb{R}^K \otimes \mathrm{w}^{(\ell)}),\quad \mathrm{v}\in\mathbb{R}^K,\quad \ell=1,\dots,N.$$

The extremal eigenvalues of

$$(\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)}) = \begin{pmatrix} (a^{(\ell)})^2+(b^{(\ell)})^2 & a^{(\ell)}b^{(\ell)} & & \\ a^{(\ell)}b^{(\ell)} & \ddots & \ddots & \\ & \ddots & (a^{(\ell)})^2+(b^{(\ell)})^2 & a^{(\ell)}b^{(\ell)} \\ & & a^{(\ell)}b^{(\ell)} & (a^{(\ell)})^2 \end{pmatrix}$$

are now estimated in terms of the Gershgorin circle theorem [Ger31]: While the minimal eigenvalue $\lambda_{\min}\big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\big)$ satisfies

$$\begin{aligned}\lambda_{\min}\big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\big) &\geqslant \min\big((a^{(\ell)})^2+(b^{(\ell)})^2-2a^{(\ell)}|b^{(\ell)}|, (a^{(\ell)})^2-a^{(\ell)}|b^{(\ell)}|\big)\\ &= \big(a^{(\ell)}-|b^{(\ell)}|\big)^2+\min\Big(0,|b^{(\ell)}|\big(a^{(\ell)}-|b^{(\ell)}|\big)\Big) = \big(a^{(\ell)}-|b^{(\ell)}|\big)^2 > 0\end{aligned}$$

by virtue of (13), $a^{(\ell)}+b^{(\ell)}=\tau d^{(\ell)}>0$, and $a^{(\ell)}\geqslant 0$, the following inequality is valid for the maximal eigenvalue:

$$\lambda_{\max}\big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\big) \leqslant (a^{(\ell)})^2+(b^{(\ell)})^2+2a^{(\ell)}|b^{(\ell)}| = \big(a^{(\ell)}+|b^{(\ell)}|\big)^2$$

Therefore, the condition number is bounded from above by

$$\mathrm{cond}_2(\mathbf{S}_K) = \frac{\max_{\ell=1,\dots,K}\sqrt{\lambda_{\max}\big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\big)}}{\min_{\ell=1,\dots,K}\sqrt{\lambda_{\min}\big((\mathrm{S}_K^{(\ell)})^\top(\mathrm{S}_K^{(\ell)})\big)}} \leqslant \frac{\max_{\ell=1,\dots,N}\big(a^{(\ell)}+|b^{(\ell)}|\big)}{\min_{\ell=1,\dots,N}\big(a^{(\ell)}-|b^{(\ell)}|\big)},$$

which proves the statement of the theorem. □

In particular, the right hand side of (21) does not depend on the number of blocked time steps $K$ and, hence, the all-at-once system does not become ill-condition for arbitrary many blocked time steps. Under moderate time-step restrictions, the above result can basically be used to show that $\mathrm{cond}_2(\mathbf{S}_K)\leqslant C(N^2+\tau^{-1})$ for some constant $C>0$ no matter how the problem is discretized in space and time.

# 5 Time-simultaneous (block-)Jacobi method

After proving that the all-at-once system of equations (11) does not become ill-conditioned as the number of blocked time steps increases, we now take a first step towards the definition and analysis of an efficient solver for this global system. For this purpose, we introduce the (block-)Jacobi method and prove that this scheme converges (monotonically) for appropriately chosen relaxation parameters. Although the converge rate is close to 1 and, hence, not satisfactory, we will see in Section 5.4 that a few iterations may suffice to significantly reduce spatial high-frequency error modes.

## 5.1 Fundamentals

By merging all temporal unknowns associated with one spatial node into a single 'macro' degree of freedom, the global system (11) can be interpreted as a space-only problem for vector-valued unknowns. This motivates the introduction of the following *damped (block-)Jacobi method* for the solution of (11):

$$\mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + \omega\mathbf{D}_K^{-1}(\mathbf{b}-\mathbf{S}_K\mathbf{u}^{(n)}) = \omega\mathbf{D}_K^{-1}\mathbf{b}+\mathbf{J}_K^{(\mathrm{Jac})}\mathbf{u}^{(n)},\quad n=0,1,\dots \tag{23}$$

Here, the vector $\mathbf{u}^{(0)}\in\mathbb{R}^{NK}$ is an adequate initial guess, $\omega>0$ denotes the (fixed) damping parameter, $\mathbf{J}_K^{(\mathrm{Jac})} := \mathbf{D}_K^{-1}(\mathbf{D}_K-\omega\mathbf{S}_K) = \mathbf{I}_K-\omega\mathbf{D}_K^{-1}\mathbf{S}_K \in\mathbb{R}^{NK\times NK}$ is the iteration matrix of the scheme, and

$\mathbf{I}_K \in \mathbb{R}^{NK\times NK}$ denotes the global identity matrix. Furthermore, the preconditioner $\mathbf{D}_K \in \mathbb{R}^{NK\times NK}$ is set to the (block-)diagonal of the 'space-only' system matrix $\mathbf{S}_K$ and does not contain any spatial couplings. More precisely, the block-matrix $\mathbf{D}_K$ is given by

$$\mathbf{D}_K = \begin{pmatrix} \tilde{\mathrm{A}} & & & \\ \tilde{\mathrm{B}} & \tilde{\mathrm{A}} & & \\ & \ddots & \ddots & \\ & & \tilde{\mathrm{B}} & \tilde{\mathrm{A}} \end{pmatrix} \in \mathbb{R}^{NK\times NK},$$

where $\tilde{\mathrm{A}} \in \mathbb{R}^{N\times N}$ and $\tilde{\mathrm{B}} \in \mathbb{R}^{N\times N}$ are the diagonal matrices associated to A and B, i.e.,

$$\tilde{\mathrm{A}} = (m_{ii} + \theta\tau d_{ii})\mathrm{I}, \quad \tilde{\mathrm{B}} = \big(-m_{ii} + (1-\theta)\tau d_{ii}\big)\mathrm{I}.$$

Note that the diagonal entries $a_{ii} = m_{ii} + \theta\tau d_{ii}$ of $\tilde{\mathrm{A}}$ are constant and positive by definition. Thus, the inverse of $\tilde{\mathrm{A}}$ is well defined and it can be easily verified that $\mathbf{D}_K^{-1} \in \mathbb{R}^{NK\times NK}$ reads

$$\mathbf{D}_K^{-1} = \begin{pmatrix} \tilde{\mathrm{A}}^{-1} & & & \\ (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})\tilde{\mathrm{A}}^{-1} & \tilde{\mathrm{A}}^{-1} & & \\ \vdots & \ddots & \ddots & \\ (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})^{K-1}\tilde{\mathrm{A}}^{-1} & \cdots & (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})\tilde{\mathrm{A}}^{-1} & \tilde{\mathrm{A}}^{-1} \end{pmatrix}. \tag{24}$$

Therefore, the iteration matrix $\mathbf{J}_K^{(\mathrm{Jac})} = \mathbf{D}_K^{-1}(\mathbf{D}_K - \omega\mathbf{S}_K)$ is defined as a product of two lower triangular block matrices and, hence, has the same structure. This property is exploited in the following section to easily determine the asymptotic rate of convergence of (23).

## 5.2 Spectral radius of Jacobi iteration matrix

While commonly convergence of the (block-)Jacobi method is guaranteed by scaling the solution update using a positive damping parameter bounded from above by unity, we now prove that this upper barrier can be slightly relaxed in terms of the CFL number $\lambda = \tau h^{-2}$.

**Theorem 5.** *The spectral radius of the (block-)Jacobi iteration matrix satisfies*

$$\mathrm{spr}(\mathbf{J}_K^{(\mathrm{Jac})}) = \mathrm{spr}(\mathrm{J}^{(\mathrm{Jac})}) = \max_{\ell=1,\dots,N} |j^{(\mathrm{Jac},\ell)}| < 1, \quad \omega \in (0,\bar{\omega}) \tag{25}$$

*for all $\theta \in [0,1]$, where $j^{(\mathrm{Jac},\ell)} = 1 - \omega a_{ii}^{-1} a^{(\ell)}$, $\ell = 1,\dots,N$, denote the eigenvalues of $\mathrm{J}^{(\mathrm{Jac})} = \mathrm{I} - \omega\tilde{\mathrm{A}}^{-1}\mathrm{A}$ and*

$$\bar{\omega} := \frac{2m_{ii} + 2\theta\tau d_{ii}}{(2-\zeta)m_{ii} + 2\theta\tau d_{ii}} > 1. \tag{26}$$

Convergence can even be guaranteed if $\omega = \bar{\omega} < 2$ by slightly modifying the proof. However, this more general result would only lengthen the notation and, hence, is omitted for the sake of simplicity.

*Proof.* To prove the statement of Theorem 5, we first note that $\mathbf{J}_K^{(\mathrm{Jac})}$ is a triangular block matrix. Therefore, its spectral radius coincides with the maximal spectral radius of the diagonal blocks. In case of the (block-) Jacobi iteration matrix, the block diagonal entries are constant and read $\mathrm{J}^{(\mathrm{Jac})} = \mathrm{I} - \omega\tilde{\mathrm{A}}^{-1}\mathrm{A}$ which implies $\mathrm{spr}(\mathbf{J}_K^{(\mathrm{Jac})}) = \mathrm{spr}(\mathrm{J}^{(\mathrm{Jac})})$. Furthermore, the spatial matrix $\mathrm{J}^{(\mathrm{Jac})}$ is symmetric and possesses the eigenvalues

$$j^{(\mathrm{Jac},\ell)} = 1 - \omega a_{ii}^{-1} a^{(\ell)} = 1 - \omega\frac{m^{(\ell)} + \theta\tau d^{(\ell)}}{m_{ii} + \theta\tau d_{ii}}, \quad \ell = 1,\dots,N.$$

Due to the fact that $m^{(\ell)}, d^{(\ell)} > 0$ for all $\ell = 1,\dots,N$, all eigenvalues are smaller than 1 no matter how $\omega > 0$ is chosen. On the other hand, the eigenvalues $j^{(\mathrm{Jac},\ell)}$ are bounded from below by $-1$ because

$$j^{(\mathrm{Jac},\ell)} = 1 - \omega\frac{m^{(\ell)} + \theta\tau d^{(\ell)}}{m_{ii} + \theta\tau d_{ii}} > 1 - \bar{\omega}\frac{(2-\zeta)m_{ii} + 2\theta\tau d_{ii}}{m_{ii} + \theta\tau d_{ii}} = 1 - 2 = -1$$

by (7) and (8) if $\omega \in (0,\bar{\omega})$. □

Therefore, the fixed point iteration (23) converges asymptotically with a rate independent of the number of blocked time steps $K$. Additionally, (moderate) overrelaxation is reasonable especially for small time increments $\tau$ and, as we will see in Section 6.4, might significantly improve the asymptotic rate of convergence of the considered two-grid algorithm.

Although the convergence of the (block-)Jacobi scheme is guaranteed by Theorem 5, this method is not a good solver for the global system (11) per se because the convergence behavior deteriorates as the mesh is refined no matter how $\omega \in (0, \bar{\omega}) \subseteq (0, 2)$ is chosen, at least when $\theta > 0$ is used.

## 5.3 Spectral norm of Jacobi iteration matrix

While Theorem 5 ensures convergence of the (block-)Jacobi scheme (23) even for relaxation parameters greater than unity, we now prove that the iterates converge monotonically, at least for relaxation parameters $\omega$ smaller than 1. This result is shown by exploiting the statement of Theorem 3 and the tensor product approach as already used in Section 4.

**Theorem 6.** *The (block-)Jacobi scheme* (23) *converges monotonically with respect to the Euclidean norm for every relaxation parameter* $\omega \in (0, 1]$ *and the iteration matrix* $\mathbf{J}_K^{(\mathrm{Jac})}$ *satisfies*

$$\sup_{\mathbf{u} \in (\mathbb{R}^K \otimes \mathrm{w}^{(\ell)}) \setminus \{\mathbf{0}\}} \frac{\left\| \mathbf{J}_K^{(\mathrm{Jac})} \mathbf{u} \right\|_2}{\|\mathbf{u}\|_2} = \|\mathrm{J}_K^{(\mathrm{Jac},\ell)}\|_2 \leqslant B^{(\ell)}, \quad \ell = 1, \ldots, N \tag{27a}$$

$$B^{(\ell)} := \max\left( \left| 1 - \omega \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} \right|, \left| 1 - \omega \frac{d^{(\ell)}}{d_{ii}} \right| \right) < 1, \tag{27b}$$

*where* $\mathrm{J}_K^{(\mathrm{Jac},\ell)} \in \mathbb{R}^{K \times K}$ *can be interpreted as the iteration matrix of the spatial Fourier mode* $\mathrm{w}^{(\ell)}$ *and is defined by*

$$\mathrm{J}_K^{(\mathrm{Jac},\ell)} := (\mathrm{D}_K)^{-1}(\mathrm{D}_K - \omega \mathrm{S}_K^{(\ell)}), \qquad \mathrm{D}_K = \begin{pmatrix} a_{ii} & & & \\ b_{ii} & a_{ii} & & \\ & \ddots & \ddots & \\ & & b_{ii} & a_{ii} \end{pmatrix} \in \mathbb{R}^{K \times K}.$$

*Proof.* Again we would like to exploit the above mentioned tensor product approach and, for this, recall that $\mathrm{w}^{(1)}, \ldots, \mathrm{w}^{(N)}$ are eigenvectors of $\mathrm{A}$, $\mathrm{B}$, $\tilde{\mathrm{A}}$, $\tilde{\mathrm{B}}$, and $\tilde{\mathrm{A}}^{-1}$. Therefore, according to (24), the (block-)Jacobi iteration matrix satisfies

$$
\begin{aligned}
\mathbf{J}_K^{(\mathrm{Jac})}\mathbf{w} &= \mathbf{D}_K^{-1}(\mathbf{D}_K-\omega\mathbf{S}_K)\mathbf{w}\\
&= \begin{pmatrix} \tilde{\mathrm{A}}^{-1} & & & \\ (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})\tilde{\mathrm{A}}^{-1} & \tilde{\mathrm{A}}^{-1} & & \\ \vdots & \ddots & \ddots & \\ (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})^{K-1}\tilde{\mathrm{A}}^{-1} & \cdots & (-\tilde{\mathrm{A}}^{-1}\tilde{\mathrm{B}})\tilde{\mathrm{A}}^{-1} & \tilde{\mathrm{A}}^{-1} \end{pmatrix}\\
&\quad\cdot \begin{pmatrix} \tilde{\mathrm{A}}-\omega\mathrm{A} & & & \\ \tilde{\mathrm{B}}-\omega\mathrm{B} & \tilde{\mathrm{A}}-\omega\mathrm{A} & & \\ & \ddots & \ddots & \\ & & \tilde{\mathrm{B}}-\omega\mathrm{B} & \tilde{\mathrm{A}}-\omega\mathrm{A} \end{pmatrix} \begin{pmatrix} v_1\mathrm{w}^{(\ell)} \\ v_2\mathrm{w}^{(\ell)} \\ \vdots \\ v_K\mathrm{w}^{(\ell)} \end{pmatrix}\\
&= \begin{pmatrix} a_{ii}^{-1}\mathrm{I} & & & \\ (-a_{ii}^{-1}b_{ii})a_{ii}^{-1}\mathrm{I} & a_{ii}^{-1}\mathrm{I} & & \\ \vdots & \ddots & \ddots & \\ (-a_{ii}^{-1}b_{ii})^{K-1}a_{ii}^{-1}\mathrm{I} & \cdots & (-a_{ii}^{-1}b_{ii})a_{ii}^{-1}\mathrm{I} & a_{ii}^{-1}\mathrm{I} \end{pmatrix}\\
&\quad\cdot \begin{pmatrix} (a_{ii}-\omega a^{(\ell)})\mathrm{I} & & & \\ (b_{ii}-\omega b^{(\ell)})\mathrm{I} & (a_{ii}-\omega a^{(\ell)})\mathrm{I} & & \\ & \ddots & \ddots & \\ & & (b_{ii}-\omega b^{(\ell)})\mathrm{I} & (a_{ii}-\omega a^{(\ell)})\mathrm{I} \end{pmatrix} \begin{pmatrix} v_1\mathrm{w}^{(\ell)} \\ v_2\mathrm{w}^{(\ell)} \\ \vdots \\ v_K\mathrm{w}^{(\ell)} \end{pmatrix}\\
&= \Big(\big((\mathrm{D}_K)^{-1}(\mathrm{D}_K-\omega\mathrm{S}_K^{(\ell)})\big)\otimes\mathrm{I}\Big)\mathbf{w} = \Big(\big((\mathrm{D}_K)^{-1}(\mathrm{D}_K-\omega\mathrm{S}_K^{(\ell)})\big)\mathrm{v}\Big)\otimes\mathrm{w}^{(\ell)}
\end{aligned}
$$

for $\mathbf{w}=\mathrm{v}\otimes\mathrm{w}^{(\ell)}\in\mathbb{R}^{NK}$, where $\mathrm{v}\in\mathbb{R}^K$ and $\ell=1,\dots,N$ are chosen arbitrarily. For this reason, we have

$$\mathbf{J}_K^{(\mathrm{Jac})}(\mathrm{v}\otimes\mathrm{w}^{(\ell)}) = (\mathrm{J}_K^{(\mathrm{Jac},\ell)}\mathrm{v})\otimes\mathrm{w}^{(\ell)} \in (\mathbb{R}^K\otimes\mathrm{w}^{(\ell)}),\quad \mathrm{v}\in\mathbb{R}^K,\quad \ell=1,\dots,N,$$

where $\mathrm{J}_K^{(\mathrm{Jac},\ell)} := (\mathrm{D}_K)^{-1}(\mathrm{D}_K-\omega\mathrm{S}_K^{(\ell)})$, and the spectral norm of $\mathbf{J}_K^{(\mathrm{Jac})}$ can be computed using

$$\|\mathbf{J}_K^{(\mathrm{Jac})}\|_2 = \max_{\ell=1,\dots,N}\|\mathbf{J}_K^{(\mathrm{Jac})}\|_{2,\mathbb{R}^K\otimes\mathrm{w}^{(\ell)}} = \max_{\ell=1,\dots,N}\big\|\mathrm{J}_K^{(\mathrm{Jac},\ell)}\big\|_2 = \max_{\ell=1,\dots,N}\big\|(\mathrm{D}_K)^{-1}(\mathrm{D}_K-\omega\mathrm{S}_K^{(\ell)})\big\|_2 \tag{28}$$

according to Lemma 2 and due to the fact that $\mathrm{w}^{(1)},\dots,\mathrm{w}^{(N)}$ form a basis of $\mathbb{R}^N$.

In the remainder of this proof, we show that the spectral norm of $\mathrm{J}_K^{(\mathrm{Jac},\ell)}$ is smaller than 1 by exploiting Theorem 3 using $\mathrm{E}=\mathrm{D}_K-\omega\mathrm{S}_K^{(\ell)}$ and $\mathrm{F}=\mathrm{D}_K$, i.e.,

$$
\begin{aligned}
e_1 &= (m_{ii}+\theta\tau d_{ii})-\omega(m^{(\ell)}+\theta\tau d^{(\ell)}), & f_1 &= m_{ii}+\theta\tau d_{ii},\\
e_2 &= \big(-m_{ii}+(1-\theta)\tau d_{ii}\big)-\omega\big(-m^{(\ell)}+(1-\theta)\tau d^{(\ell)}\big), & f_2 &= -m_{ii}+(1-\theta)\tau d_{ii}.
\end{aligned} \tag{29}
$$

This theorem can be employed because the requirement $|f_2|<|f_1|$ is satisfied whenever the CFL-like condition (10) holds. Indeed, the value of $f_2^2-f_1^2$ is equal to

$$
\begin{aligned}
f_2^2-f_1^2 &= \big(-m_{ii}+(1-\theta)\tau d_{ii}\big)^2-(m_{ii}+\theta\tau d_{ii})^2\\
&= m_{ii}^2-2(1-\theta)\tau m_{ii}d_{ii}+(1-\theta)^2\tau^2 d_{ii}^2-m_{ii}^2-2\theta\tau m_{ii}d_{ii}-\theta^2\tau^2 d_{ii}^2\\
&= -2\tau m_{ii}d_{ii}+(1-2\theta)\tau^2 d_{ii}^2 = -\tau d_{ii}\underbrace{\big(2m_{ii}-(1-2\theta)\tau d_{ii}\big)}_{\geqslant(2-\zeta)m_{ii}>0\text{ by (10)}}<0.
\end{aligned} \tag{30}
$$

Furthermore, it is easy to verify that the value of $B^{(\ell)}$ coincides with the bound of (20) for the quantities as defined in (29). To complete the proof, it suffices to show that both expressions involved in the definition of $B^{(\ell)}$ are smaller than 1: For $\eta \geqslant 0$, this estimate is true because

$$\begin{aligned}(e_1+e_2)^2-(f_1+f_2)^2 &= (\tau d_{ii}-\omega\tau d^{(\ell)})^2-(\tau d_{ii})^2\\ &= -2\omega\tau^2 d_{ii}d^{(\ell)}+\omega^2\tau^2(d^{(\ell)})^2=\omega\tau^2 d^{(\ell)}(-2d_{ii}+\omega d^{(\ell)})<0\end{aligned}$$

by (7). On the other hand, the inequality $|e_1-e_2|<|f_1-f_2|$ is satisfied because

$$\begin{aligned}&(e_1-e_2)^2-(f_1-f_2)^2\\ &\quad=\big(2m_{ii}-2\omega m^{(\ell)}-(1-2\theta)\tau(d_{ii}-\omega d^{(\ell)})\big)^2-\big(2m_{ii}-(1-2\theta)\tau d_{ii}\big)^2\\ &\quad=\omega\big(2m^{(\ell)}-(1-2\theta)\tau d^{(\ell)}\big)\Big(-2\big(2m_{ii}-(1-2\theta)\tau d_{ii}\big)+\omega\big(2m^{(\ell)}-(1-2\theta)\tau d^{(\ell)}\big)\Big)\\ &\quad=\omega\underbrace{\big(2m^{(\ell)}-(1-2\theta)\tau d^{(\ell)}\big)}_{>0\text{ by }(13)}\Big(2\underbrace{\big(-\zeta m_{ii}+(1-2\theta)\tau d_{ii}\big)}_{\leqslant 0\text{ by }(10)}-2\underbrace{\big((2-\zeta)m_{ii}-\omega m^{(\ell)}\big)}_{\geqslant 0\text{ by }(8)}-\omega\underbrace{(1-2\theta)\tau d^{(\ell)}}_{>0\text{ by }\theta<\frac12}\Big)<0\end{aligned}$$

for $\theta<\frac12$ while the expression is negative for $\theta\geqslant\frac12$ due to

$$\begin{aligned}(e_1-e_2)^2-(f_1-f_2)^2=\omega&\overbrace{\big(2m^{(\ell)}-(1-2\theta)\tau d^{(\ell)}\big)}^{>0\text{ by }(13)}\\ &\cdot\Big(-\underbrace{2\zeta m_{ii}}_{>0}+\underbrace{(1-2\theta)}_{\leqslant 0}\tau\underbrace{\big(2d_{ii}-\omega d^{(\ell)}\big)}_{>0\text{ by }(7)}-2\underbrace{\big((2-\zeta)m_{ii}-\omega m^{(\ell)}\big)}_{\geqslant 0\text{ by }(8)}\Big)<0.\end{aligned}$$

Therefore, the spectral norm $\|\mathrm{J}_K^{(\mathrm{Jac},\ell)}\|_2$ is bounded from above by 1 and the (block-)Jacobi scheme converges monotonically by (28). □

## 5.4 Smoothing behavior

In the previous section, Theorem 3 was only employed to show the monotone convergence of the (block-)Jacobi scheme. However, the theorem offers the possibility to perform more detailed investigations of the convergence behavior by considering individual (spatial) Fourier modes separately. These studies show that high-frequency error modes are significantly damped for an appropriately chosen relaxation parameter and motivate the use of multigrid techniques to solve (11).

To analyze the smoothing property of the (block-)Jacobi scheme, we first consider the influence of $\omega$ on the bounds for the error reduction of each (spatial) Fourier mode as introduced in Theorem 6.

**Example 7.** The bounds $B^{(\ell)}$ of Theorem 6 are not only bounded by 1, but also guarantee a mesh-independent reduction of high-frequency error modes for an appropriately chosen relaxation parameter. Figure 1 illustrates the influence of $\omega$ on the bounds $B^{(\ell)}$ for a finite element discretization whenever $s_\ell^2\geqslant\frac12$. Although the choice of $\lambda=\tau h^{-2}=\frac56$ for $\theta\geqslant\frac12$ is practically of minor interest, this setup is considered to present the influence of both arguments occurring in the definition of $B^{(\ell)}$. Furthermore, the potentially 'optimal' relaxation parameter $\omega_0$ for smoothing high-frequency parts of the error is highlighted. In what follows, this parameter will be investigated in more detail and used in the two-grid algorithm presented in Section 6.3.

In the following theorem, an explicit formula for $\omega_0$ is determined and, based on this choice, an upper bound for $B^{(\ell)}$ is derived for every $\ell=1,\dots,N$.

**Theorem 8.** *If the relaxation parameter $\omega$ coincides with*

$$\omega_0=\max\Big(\frac23,\frac{2m_{ii}-(1-2\theta)\tau d_{ii}}{(2+\zeta)m_{ii}-2(1-2\theta)\tau d_{ii}}\Big)=\max\Big(\frac23,\frac{(2-\zeta)m_{ii}+\kappa}{(2-\zeta)m_{ii}+2\kappa}\Big)\leqslant 1, \tag{31}$$

*then high-frequency error modes are damped at least with the factor*

$$B^{(\ell)}\leqslant E^{(\mathrm{Jac},\ell)}:=\max\Big(\frac13,\frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii}-2(1-2\theta)\tau d_{ii}}\Big)=\max\Big(\frac13,\frac{(2-\zeta)m_{ii}}{(2-\zeta)m_{ii}+2\kappa}\Big),$$
$$\ell=1,\dots,N\ \ s.t.\ \ d^{(\ell)}>d_{ii}. \tag{32}$$

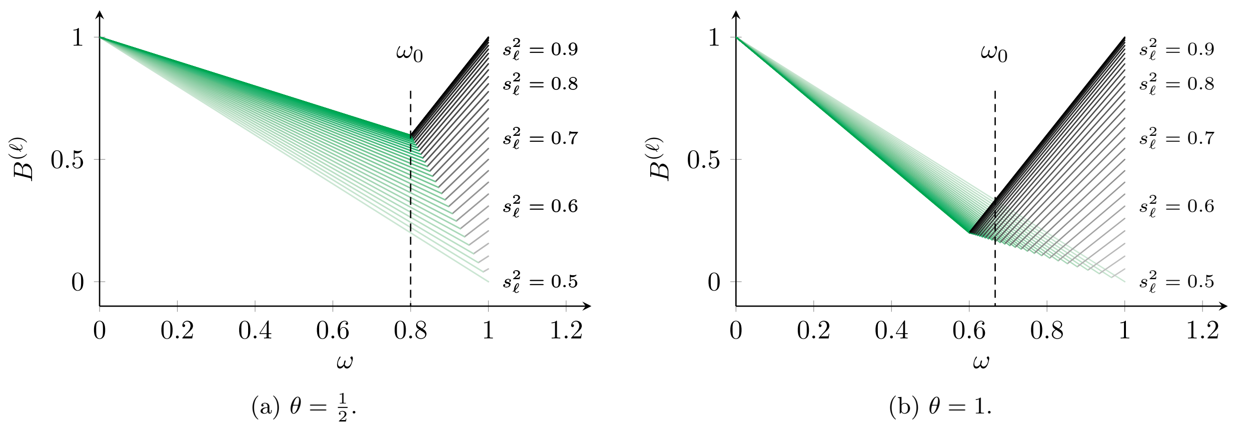



Figure 1: Influence of damping parameter $\omega$ on bound $B^{(\ell)}$ for high-frequency modes of a finite element discretization using $\lambda = \tau h^{-2} = \frac{5}{6}$. Graphs are highlighted in green whenever maximum in (27b) attains value of first argument. 'Optimal' relaxation parameter is highlighted by $\omega_0$.

*On the other hand, low-frequency modes are scaled with*

$$B^{(\ell)} = 1 - \omega d_{ii}^{-1} d^{(\ell)}, \quad \ell = 1, \dots, N \text{ s.t. } d^{(\ell)} \leqslant d_{ii} \tag{33}$$

*no matter how $\omega \in (0, 1]$ is chosen.*

*Proof.* The proof of this theorem can be found in the appendix. □

The numerical examples presented in Section 6.4 indicate that the damping parameter $\omega_0$ (approximately) minimizes the spectral norm of the two-grid iteration matrix in the limit $K \to \infty$ and, hence, might be asymptotically 'optimal', at least for a few smoothing steps. Therefore, this choice of $\omega$ is used in what follows if not mentioned otherwise and we set

$$E^{(\text{Jac},\ell)} := 1 - \omega_0 d_{ii}^{-1} d^{(\ell)}, \quad \ell = 1, \dots, N \text{ s.t. } d^{(\ell)} \leqslant d_{ii}. \tag{34}$$

*Remark* 9. In the context of finite differences and $\theta \geqslant \frac{1}{2}$, the damping parameter $\omega_0$ coincides with $\frac{2}{3}$ no matter how $N$ and $\tau$ are chosen. Then high-frequency error modes, that is, if $d^{(\ell)} > d_{ii}$ is satisfied, are damped with $B^{(\ell)} \leqslant E^{(\text{Jac},\ell)} = \frac{1}{3}$.

For a finite element discretization, the relaxation parameter $\omega_0 \in [\frac{2}{3}, \frac{4}{5}]$ guarantees $E^{(\text{Jac},\ell)} \leqslant \frac{3}{5}$ if $\theta \geqslant \frac{1}{2}$ and $d^{(\ell)} > d_{ii}$. While in the best case $E^{(\text{Jac},\ell)} = \frac{1}{3}$ for $\theta > \frac{1}{2}$, the smoothing behavior deteriorates if $\lambda = \tau h^{-2}$ decreases. For the Crank-Nicolson scheme, i.e., $\theta = \frac{1}{2}$, the 'optimal' damping parameter reads $\omega_0 = \frac{4}{5}$ and guarantees $E^{(\text{Jac},\ell)} = \frac{3}{5}$ for all choices of $N$ and $\tau$ if $d^{(\ell)} > d_{ii}$.

In the case of $\theta < \frac{1}{2}$, the above theorem does not suffice to guarantee a mesh-independent value of $E^{(\text{Jac},\ell)} < 1$ for high-frequency error modes if equality holds in the CFL-like condition (10), i.e., $\kappa = 0$.

*Remark* 10. For a sequential simulation, that is, $K = 1$, excellent damping of high-frequency error modes is obtained for

$$\omega_{\text{seq}} = \frac{2m_{ii} + 2\theta\tau d_{ii}}{(1+\zeta)m_{ii} + 3\theta\tau d_{ii}} \in \left(\tfrac{2}{3}, 2(1+\zeta)^{-1}\right).$$

However, the 'optimal' damping parameter for $K = 1$ does *not* minimize the spectral norm of the two-grid iteration matrix for $K > 1$ as we will see in Section 6.4.

# 6 Time-simultaneous two-grid solver

In the previous section, the (block-)Jacobi scheme for the time-simultaneous system was introduced and its smoothing behavior for high-frequency (spatial) error modes was analyzed. The results stated in Theorem 8 motivate the use of spatial multigrid techniques for solution of the all-at-once problem. Therefore, this section is devoted to the presentation of a two-grid solver and investigations regarding corresponding convergence rates.

## 6.1 Fundamentals of coarse grid correction

To define the two-grid solver, let us first introduce the coarse grid correction based on commonly used spatial coarsening techniques. For this purpose, the number of (inner) fine grid nodes is assumed to be odd and at least equal to 3, i.e., $N \in 2\mathbb{N}+1$. Then, based on a uniform coarsening/refinement strategy, the mesh size of the coarse grid reads $\bar{h} = 2h = (\bar{N}+1)^{-1}$, where the number of spatial unknowns corresponding to the coarse mesh is given by $\bar{N} = \frac{N-1}{2}$. Therefore, the system matrix of the all-at-once coarse grid problem exploiting the same time increment $\tau$ as used in (11) reads

$$\bar{\mathbf{S}}_K := \begin{pmatrix} \bar{\mathrm{A}} & & & \\ \bar{\mathrm{B}} & \bar{\mathrm{A}} & & \\ & \ddots & \ddots & \\ & & \bar{\mathrm{B}} & \bar{\mathrm{A}} \end{pmatrix}, \tag{35}$$

where $\bar{\mathrm{A}}, \bar{\mathrm{B}} \in \mathbb{R}^{\bar{N}\times\bar{N}}$ are defined by

$$\bar{\mathrm{A}} := \bar{\mathrm{M}} + \theta\tau\bar{\mathrm{D}}, \quad \bar{\mathrm{B}} := -\bar{\mathrm{M}} + (1-\theta)\tau\bar{\mathrm{D}}$$

and the matrices $\bar{\mathrm{M}} \in \mathbb{R}^{\bar{N}\times\bar{N}}$ and $\bar{\mathrm{D}} \in \mathbb{R}^{\bar{N}\times\bar{N}}$ denote the mass matrix and discrete counterpart of the negative laplacian discretized on the coarse mesh using finite differences or finite elements. As stated in Section 2, these spatial matrices possess the same set of eigenvectors

$$\bar{\mathrm{w}}^{(\ell)} = \sqrt{2(\bar{N}+1)^{-1}}\Big(\sin\big(\pi k\ell(\bar{N}+1)^{-1}\big)\Big)_{k=1}^{\bar{N}} = \sqrt{4(N+1)^{-1}}\Big(\sin\big(2\pi k\ell(N+1)^{-1}\big)\Big)_{k=1}^{\bar{N}}, \quad \ell = 1,\dots,\bar{N}$$

associated with the eigenvalues

$$\begin{aligned} \bar{m}^{(\ell)} &= \tfrac{2}{3}(\bar{N}+1)^{-1}\Big(\tfrac{3}{2} - \sin^2\big(\tfrac{\pi}{2}\ell(\bar{N}+1)^{-1}\big)\Big) = \tfrac{4}{3}(N+1)^{-1}\Big(\tfrac{3}{2} - \sin^2\big(\pi\ell(N+1)^{-1}\big)\Big) \\ &= 2m_{ii}\Big(\tfrac{3}{2} - 4\sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\cos^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\Big) = m_{ii}(3 - 8s_\ell^2c_\ell^2), \end{aligned} \tag{36a}$$

$$\begin{aligned} \bar{d}^{(\ell)} &= 4(\bar{N}+1)\sin^2\big(\tfrac{\pi}{2}\ell(\bar{N}+1)^{-1}\big) = 2(N+1)\sin^2\big(\pi\ell(N+1)^{-1}\big) \\ &= 8(N+1)\sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\cos^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) = 4d_{ii}s_\ell^2c_\ell^2 \end{aligned} \tag{36b}$$

for finite elements while $\bar{m}^{(\ell)} = 1$ and

$$\begin{aligned} \bar{d}^{(\ell)} &= 4(\bar{N}+1)^2\sin^2\big(\tfrac{\pi}{2}\ell(\bar{N}+1)^{-1}\big) = (N+1)^2\sin^2\big(\pi\ell(N+1)^{-1}\big) \\ &= 4(N+1)^2\sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big)\cos^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) = 2d_{ii}s_\ell^2c_\ell^2 \end{aligned} \tag{37}$$

in the context of a finite difference approximation. In particular, the eigenvalues satisfy

$$(2-\zeta)^{-1}m^{(\ell)} \leqslant m_{ii} \leqslant \bar{m}^{(\ell)} \leqslant \zeta^{-1}m^{(\ell)}, \qquad \ell = 1,\dots,\bar{N}, \tag{38}$$

$$0 \leqslant \bar{d}^{(\ell)} = 2\zeta^{-1}s_\ell^2c_\ell^2d_{ii} = \zeta^{-1}c_\ell^2d^{(\ell)} = \zeta^{-1}s_\ell^2d^{(N+1-\ell)} \leqslant (2\zeta)^{-1}d_{ii}, \quad \ell = 1,\dots,\bar{N} \tag{39}$$

due to the fact that $d^{(\ell)} = 2s_\ell^2d_{ii}$ and $d^{(N+1-\ell)} = 2c_\ell^2d_{ii}$ for all $\ell = 1,\dots,\bar{N}$.

Next, we introduce the spatial grid transfer operators which are given by the commonly used prolongation and restriction operators $\mathrm{P} \in \mathbb{R}^{N \times \bar{N}}$ and $\mathrm{R} \in \mathbb{R}^{\bar{N} \times N}$, respectively,

$$\mathrm{P} = \frac{1}{2} \begin{pmatrix} 1 & & & & \\ 2 & & & & \\ 1 & 1 & & & \\ & 2 & & & \\ & & \ddots & & \\ & & & 2 & \\ & & & 1 & 1 \\ & & & & 2 \\ & & & & 1 \end{pmatrix}, \qquad \mathrm{R} = (2\zeta)^{-1}\mathrm{P}^\top = (4\zeta)^{-1} \begin{pmatrix} 1 & 2 & 1 & & & & \\ & & 1 & 2 & 1 & & \\ & & & \ddots & & \ddots & \\ & & & & 1 & 2 & 1 \end{pmatrix}.$$

These matrices satisfy [Hac13, Section 2.4]

$$\mathrm{P}\bar{\mathrm{w}}^{(\bar{N}+1)} = 0, \qquad \mathrm{P}\bar{\mathrm{w}}^{(\ell)} = \sqrt{2}c_\ell^2 \mathrm{w}^{(\ell)} - \sqrt{2}s_\ell^2 \mathrm{w}^{(N+1-\ell)}, \qquad \ell = 1, \dots, \bar{N}, \tag{40a}$$

$$\mathrm{R}\mathrm{w}^{(\bar{N}+1)} = 0, \quad \mathrm{R}\mathrm{w}^{(\ell)} = \sqrt{2}c_\ell^2 \bar{\mathrm{w}}^{(\ell)}, \quad \mathrm{R}\mathrm{w}^{(N+1-\ell)} = -\sqrt{2}s_\ell^2 \bar{\mathrm{w}}^{(\ell)}, \quad \ell = 1, \dots, \bar{N} \tag{40b}$$

using the quantities $s_\ell$ and $c_\ell$ as defined in (6)

$$s_\ell^2 = \sin^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) \in (0, \tfrac{1}{2}], \quad c_\ell^2 = \cos^2\big(\tfrac{\pi}{2}\ell(N+1)^{-1}\big) \in [\tfrac{1}{2}, 1), \qquad \ell = 1, \dots, \bar{N}+1.$$

Then the iteration matrix of the coarse grid correction reads

$$\mathbf{J}_K^{(\mathrm{Cor})} := \mathbf{I}_K - (\mathrm{I}_K \otimes \mathrm{P})\bar{\mathbf{S}}_K^{-1}(\mathrm{I}_K \otimes \mathrm{R})\mathbf{S}_K,$$

where $\mathrm{I}_K \in \mathbb{R}^{K \times K}$ is the (temporal) identity matrix. It is easy to verify that $\mathbf{J}_K^{(\mathrm{Cor})}$ is a lower triangular block matrix possessing the constant diagonal entries

$$\mathrm{J}^{(\mathrm{Cor})} := \mathrm{I} - \mathrm{P}\bar{\mathrm{A}}^{-1}\mathrm{R}\mathrm{A}$$

due to the fact that $\bar{\mathbf{S}}_K$ and $\mathbf{S}_K$ are triangular block matrices and, hence, the inverse of $\bar{\mathbf{S}}_K$ also possesses this structure as observed in Section 5.1 for $\mathbf{D}_K^{-1}$. Furthermore, the iteration matrix of the coarse grid correction satisfies

$$\mathrm{J}^{(\mathrm{Cor})}\mathrm{span}(\mathrm{w}^{(\ell)}, \mathrm{w}^{(N+1-\ell)}) \subseteq \mathrm{span}(\mathrm{w}^{(\ell)}, \mathrm{w}^{(N+1-\ell)}), \qquad \ell = 1, \dots, \bar{N}+1 \tag{41}$$

$$\mathbf{J}_K^{(\mathrm{Cor})}(\mathbb{R}^K \otimes \mathrm{w}^{(\ell)} + \mathbb{R}^K \otimes \mathrm{w}^{(N+1-\ell)}) \subseteq (\mathbb{R}^K \otimes \mathrm{w}^{(\ell)} + \mathbb{R}^K \otimes \mathrm{w}^{(N+1-\ell)}), \quad \ell = 1, \dots, \bar{N}+1 \tag{42}$$

by virtue of (40), which will be important in what follows to estimate the spectral radius and spectral norm of the two-grid iteration matrix

$$\mathbf{J}_K^{(\mathrm{TG})} := (\mathbf{J}_K^{(\mathrm{Jac})})^{\nu_1}\mathbf{J}_K^{(\mathrm{Cor})}(\mathbf{J}_K^{(\mathrm{Jac})})^{\nu_2},$$

where $\nu_1 \in \mathbb{N}_0$ and $\nu_2 \in \mathbb{N}_0$ denote the number of pre- and post-smoothing steps, respectively. As we will see, a few smoothing steps will suffice to significantly reduce the overall error if the relaxation parameter of $\mathbf{J}_K^{(\mathrm{Jac})}$ is chosen appropriately. For this purpose, we consider the case $\omega = \omega_0$ if not mentioned otherwise, which results in great reductions of (spatial) high-frequency error modes as observed in Section 5.4.

## 6.2 Spectral radius of two-grid iteration matrix

We begin with the analysis of the two-grid solver

$$\begin{cases} u^{(n+1,0)} = u^{(n)}, & \\ \mathbf{u}^{(n+1,m+1)} = \mathbf{u}^{(n+1,m)} + \omega\mathbf{D}_K^{-1}(\mathbf{b} - \mathbf{S}_K\mathbf{u}^{(n+1,m)}), & m = 0, 1, \dots, \nu_1 - 1, \\ \mathbf{u}^{(n+1,\nu_1+1)} = \mathbf{u}^{(n+1,\nu_1)} + (\mathrm{I}_K \otimes \mathrm{P})\bar{\mathbf{S}}_K^{-1}(\mathrm{I}_K \otimes \mathrm{R})(\mathbf{b} - \mathbf{S}_K\mathbf{u}^{(n+1,\nu_1)}), & \\ \mathbf{u}^{(n+1,\nu_1+m+2)} = \mathbf{u}^{(n+1,\nu_1+m+1)} + \omega\mathbf{D}_K^{-1}(\mathbf{b} - \mathbf{S}_K\mathbf{u}^{(n+1,\nu_1+m+1)}), & m = 0, 1, \dots, \nu_2 - 1, \\ u^{(n+1)} = u^{(n+1,\nu_1+\nu_2+1)}, & \end{cases}$$

$$n = 0, 1, \dots \tag{43}$$

by proving that the iterates $\mathbf{u}^{(n+1)}$ converge to the exact solution no matter how the relaxation parameter $\omega \in (0, \bar{\omega})$ and the initial guess $\mathbf{u}^{(0)} \in \mathbb{R}^{NK}$ are chosen. For this purpose, it is shown that the spectral radius of the iteration matrix $\mathbf{J}_K^{(\mathrm{TG})}$ is smaller than 1. This property can be verified by exploiting the identity

$$\operatorname{spr}(\mathbf{J}_K^{(\mathrm{TG})}) = \operatorname{spr}\big((\mathrm{J}^{(\mathrm{Jac})})^{\nu_1}\mathrm{J}^{(\mathrm{Cor})}(\mathrm{J}^{(\mathrm{Jac})})^{\nu_2}\big) = \operatorname{spr}\big(\mathrm{J}^{(\mathrm{Cor})}(\mathrm{J}^{(\mathrm{Jac})})^{\nu}\big), \quad \nu = \nu_1 + \nu_2, \tag{44}$$

which is valid because $\mathbf{J}_K^{(\mathrm{TG})}$ is a triangular block matrix with constant diagonal entries

$$\mathrm{J}^{(\mathrm{TG})} := (\mathrm{J}^{(\mathrm{Jac})})^{\nu_1}\mathrm{J}^{(\mathrm{Cor})}(\mathrm{J}^{(\mathrm{Jac})})^{\nu_2} \in \mathbb{R}^{N\times N}$$

and the spectral radius of a product of matrices is invariant under cyclic permutations. Recalling that $\mathrm{J}^{(\mathrm{Jac})} = \mathrm{I} - \omega\tilde{\mathrm{A}}^{-1}\mathrm{A}$ is a symmetric matrix possessing the orthogonal eigenvectors $\mathrm{w}^{(1)}, \ldots, \mathrm{w}^{(N)}$ associated with the eigenvalues $j^{(\mathrm{Jac},1)}, \ldots, j^{(\mathrm{Jac},N)}$ as introduced in Theorem 5, we find that

$$\operatorname{spr}(\mathbf{J}_K^{(\mathrm{TG})}) = \max_{\ell=1,\ldots,\bar{N}+1} \operatorname{spr}_{\operatorname{span}(\mathrm{w}^{(\ell)},\mathrm{w}^{(N+1-\ell)})}\big(\mathrm{J}^{(\mathrm{Cor})}(\mathrm{J}^{(\mathrm{Jac})})^{\nu}\big) = \max_{\ell=1,\ldots,\bar{N}+1} \operatorname{spr}\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^{\nu}\big) \tag{45}$$

by Lemma 2 and statement (41), where the matrices $\mathrm{J}^{(\mathrm{Cor},\ell)}, \mathrm{J}^{(\mathrm{Jac},\ell)} \in \mathbb{R}^{2\times 2}$ are defined by

$$\begin{aligned}
\mathrm{J}^{(\mathrm{Cor},\ell)} &:= \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} - \begin{pmatrix} \sqrt{2}c_\ell^2 \\ -\sqrt{2}s_\ell^2 \end{pmatrix} (\bar{a}^{(\ell)})^{-1} \begin{pmatrix} \frac{\sqrt{2}}{2\zeta}c_\ell^2 & -\frac{\sqrt{2}}{2\zeta}s_\ell^2 \end{pmatrix} \begin{pmatrix} a^{(\ell)} & \\ & a^{(N+1-\ell)} \end{pmatrix} \\
&= \begin{pmatrix} 1 - \zeta^{-1}c_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(\ell)} & \zeta^{-1}s_\ell^2c_\ell^2(\bar{a}^{(\ell)})^{-1}a^{(N+1-\ell)} \\ \zeta^{-1}s_\ell^2c_\ell^2(\bar{a}^{(\ell)})^{-1}a^{(\ell)} & 1 - \zeta^{-1}s_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(N+1-\ell)} \end{pmatrix}, \\
\mathrm{J}^{(\mathrm{Jac},\ell)} &:= \begin{pmatrix} j^{(\mathrm{Jac},\ell)} & \\ & j^{(\mathrm{Jac},N+1-\ell)} \end{pmatrix}
\end{aligned}$$

for all $\ell = 1, \ldots, \bar{N}$ while

$$\mathrm{J}^{(\mathrm{Cor},\bar{N}+1)} = 1, \quad \mathrm{J}^{(\mathrm{Jac},\bar{N}+1)} = j^{(\mathrm{Jac},\bar{N}+1)}.$$

Obviously, we have

$$\operatorname{spr}\big(\mathrm{J}^{(\mathrm{Cor},\bar{N}+1)}(\mathrm{J}^{(\mathrm{Jac},\bar{N}+1)})^{\nu}\big) = |j^{(\mathrm{Jac},\bar{N}+1)}|^{\nu} < 1$$

if $\omega \in (0, \bar{\omega})$ and $\nu \in \mathbb{N}$ by Theorem 5. The following theorem guarantees that $\operatorname{spr}\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^{\nu}\big) < 1$ is also valid for $\ell = 1, \ldots, \bar{N}$ no matter if finite elements or finite differences are used to discretize the heat equation in space.

**Theorem 11.** *The iterates of the two-grid method* (43) *converge to the exact solution of* (11) *for any relaxation parameter* $\omega \in (0, \bar{\omega})$ *and number of smoothing steps* $\nu = \nu_1 + \nu_2 \in \mathbb{N}$.

*Proof.* A detailed proof can be found in the appendix. □

For the sake of brevity, we will not go into detail about the derivation of explicit (and sharp) bounds for the spectral radius of the two-grid iteration matrix. Instead, the following section deals with estimates for its spectral norm, which shows that the iterates of the two-grid scheme monotonically converge to the exact solution with respect to the Euclidean norm for the damping parameter $\omega_0$.

## 6.3 Spectral norm of two-grid iteration matrix

Inspired by the observation made in (42), the tensor product approach can also be exploited to estimate the spectral norm of the two-grid iteration matrix using

$$\|\mathbf{J}_K^{(\mathrm{TG})}\|_2 = \max_{\ell=1,\ldots,\bar{N}+1} \|\mathbf{J}_K^{(\mathrm{TG})}\|_{2,\mathbb{R}^K\otimes\mathrm{w}^{(\ell)}+\mathbb{R}^K\otimes\mathrm{w}^{(N+1-\ell)}} \tag{46}$$

by virtue of Lemma 2. To simplify the expression on the right hand side of (46), we first note that the iteration matrix of the coarse grid correction satisfies

$$\begin{aligned}\mathbf{J}_K^{(\mathrm{Cor})}(\mathrm{v}\otimes\mathrm{w}^{(\bar N+1)}) &= \big(\mathbf{I}_K-(\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}(\mathrm{I}_K\otimes\mathrm{R})\mathbf{S}_K\big)(\mathrm{v}\otimes\mathrm{w}^{(\bar N+1)})\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\bar N+1)})-\big((\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}(\mathrm{I}_K\otimes\mathrm{R})\big)\big((\mathrm{S}_K^{(\bar N+1)}\mathrm{v})\otimes\mathrm{w}^{(\bar N+1)}\big)\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\bar N+1)})-\big((\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}\big)\big((\mathrm{S}_K^{(\bar N+1)}\mathrm{v})\otimes\underbrace{(\mathrm{R}\mathrm{w}^{(\bar N+1)})}_{=0}\big)\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\bar N+1)}) = (\mathrm{J}_K^{(\mathrm{Cor},\bar N+1)}\mathrm{v})\otimes\mathrm{w}^{(\bar N+1)},\quad \mathrm{v}\in\mathbb{R}^K\end{aligned}$$

by (22) and (40), where $\mathrm{J}_K^{(\mathrm{Cor},\bar N+1)}=\mathrm{I}_K\in\mathbb{R}^{K\times K}$. Similarly, the Fourier modes $\mathrm{w}^{(1)},\ldots,\mathrm{w}^{(\bar N)}$ satisfy

$$\begin{aligned}\mathbf{J}_K^{(\mathrm{Cor})}(\mathrm{v}\otimes\mathrm{w}^{(\ell)}) &= \big(\mathbf{I}_K-(\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}(\mathrm{I}_K\otimes\mathrm{R})\mathbf{S}_K\big)(\mathrm{v}\otimes\mathrm{w}^{(\ell)})\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\ell)})-\big((\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}\big)\big((\mathrm{S}_K^{(\ell)}\mathrm{v})\otimes(\mathrm{R}\mathrm{w}^{(\ell)})\big)\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\ell)})-\tfrac{\sqrt2}{2\zeta}c_\ell^2\big((\mathrm{I}_K\otimes\mathrm{P})\bar{\mathbf{S}}_K^{-1}\big)\big((\mathrm{S}_K^{(\ell)}\mathrm{v})\otimes(\bar{\mathrm{w}}^{(\ell)})\big)\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\ell)})-\tfrac{\sqrt2}{2\zeta}c_\ell^2\Big(\big((\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\mathrm{v}\big)\otimes(\mathrm{P}\bar{\mathrm{w}}^{(\ell)})\Big)\\ &= (\mathrm{v}\otimes\mathrm{w}^{(\ell)})-\zeta^{-1}c_\ell^4\Big(\big((\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\mathrm{v}\big)\otimes\mathrm{w}^{(\ell)}\Big)+\zeta^{-1}s_\ell^2c_\ell^2\Big(\big((\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\mathrm{v}\big)\otimes\mathrm{w}^{(N+1-\ell)}\Big)\\ &= \Big(\big(\mathrm{I}_K-\zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\big)\mathrm{v}\Big)\otimes\mathrm{w}^{(\ell)}+\Big(\big(\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\big)\mathrm{v}\Big)\otimes\mathrm{w}^{(N+1-\ell)}\\ &= \big(\mathrm{J}_{K,11}^{\mathrm{Cor},\ell}\mathrm{v}\big)\otimes\mathrm{w}^{(\ell)}+\big(\mathrm{J}_{K,21}^{\mathrm{Cor},\ell}\mathrm{v}\big)\otimes\mathrm{w}^{(N+1-\ell)},\\ \mathbf{J}_K^{(\mathrm{Cor})}(\mathrm{v}\otimes\mathrm{w}^{(N+1-\ell)}) &= \Big(\big(\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\big)\mathrm{v}\Big)\otimes\mathrm{w}^{(\ell)}\\ &\quad+\Big(\big(\mathrm{I}_K-\zeta^{-1}s_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\big)\mathrm{v}\Big)\otimes\mathrm{w}^{(N+1-\ell)}\\ &= \big(\mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\mathrm{v}\big)\otimes\mathrm{w}^{(\ell)}+\big(\mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\mathrm{v}\big)\otimes\mathrm{w}^{(N+1-\ell)},\end{aligned}$$

for all $\ell=1,\ldots,\bar N$ and $\mathrm{v}\in\mathbb{R}^K$, where the auxiliary matrices $\mathrm{J}_{K,11}^{\mathrm{Cor},\ell},\mathrm{J}_{K,12}^{\mathrm{Cor},\ell},\mathrm{J}_{K,21}^{\mathrm{Cor},\ell},\mathrm{J}_{K,22}^{\mathrm{Cor},\ell},\bar{\mathrm{S}}_K^{(\ell)}\in\mathbb{R}^{K\times K}$ read

$$\begin{aligned}\mathrm{J}_{K,11}^{\mathrm{Cor},\ell}&=\mathrm{I}_K-\zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}, & \mathrm{J}_{K,12}^{\mathrm{Cor},\ell}&=\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)},\\ \mathrm{J}_{K,21}^{\mathrm{Cor},\ell}&=\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}, & \mathrm{J}_{K,22}^{\mathrm{Cor},\ell}&=\mathrm{I}_K-\zeta^{-1}s_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)},\end{aligned}\qquad \bar{\mathrm{S}}_K^{(\ell)}=\begin{pmatrix}\bar a^{(\ell)} & & & \\ \bar b^{(\ell)} & \bar a^{(\ell)} & & \\ & \ddots & \ddots & \\ & & \bar b^{(\ell)} & \bar a^{(\ell)}\end{pmatrix}$$

while $\bar a^{(\ell)}=\bar m^{(\ell)}+\theta\tau\bar d^{(\ell)}$ and $\bar b^{(\ell)}=-\bar m^{(\ell)}+(1-\theta)\tau\bar d^{(\ell)}$ are the eigenvalues of the spatial coarse-grid matrices $\bar{\mathrm{A}}$ and $\bar{\mathrm{B}}$, respectively. Therefore, the iteration matrix $\mathbf{J}_K^{(\mathrm{Cor})}$ satisfies

$$\begin{aligned}&(\mathrm{v}_1\otimes\mathrm{w}^{(\ell)}+\mathrm{v}_2\otimes\mathrm{w}^{(N+1-\ell)})^\top\mathbf{J}_K^{(\mathrm{Cor})}(\mathrm{v}_1\otimes\mathrm{w}^{(\ell)}+\mathrm{v}_2\otimes\mathrm{w}^{(N+1-\ell)})\\ &\quad=(\mathrm{v}_1\otimes\mathrm{w}^{(\ell)}+\mathrm{v}_2\otimes\mathrm{w}^{(N+1-\ell)})^\top\Big(\big(\mathrm{J}_{K,11}^{\mathrm{Cor},\ell}\mathrm{v}_1\big)\otimes\mathrm{w}^{(\ell)}+\big(\mathrm{J}_{K,21}^{\mathrm{Cor},\ell}\mathrm{v}_1\big)\otimes\mathrm{w}^{(N+1-\ell)}\Big)\\ &\qquad+(\mathrm{v}_1\otimes\mathrm{w}^{(\ell)}+\mathrm{v}_2\otimes\mathrm{w}^{(N+1-\ell)})^\top\Big(\big(\mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\mathrm{v}_2\big)\otimes\mathrm{w}^{(\ell)}+\big(\mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\mathrm{v}_2\big)\otimes\mathrm{w}^{(N+1-\ell)}\Big)\\ &\quad=\mathrm{v}_1^\top\mathrm{J}_{K,11}^{\mathrm{Cor},\ell}\mathrm{v}_1+\mathrm{v}_2^\top\mathrm{J}_{K,21}^{\mathrm{Cor},\ell}\mathrm{v}_1+\mathrm{v}_1^\top\mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\mathrm{v}_2+\mathrm{v}_2^\top\mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\mathrm{v}_2\\ &\quad=\begin{pmatrix}\mathrm{v}_1\\ \mathrm{v}_2\end{pmatrix}^\top\begin{pmatrix}\mathrm{J}_{K,11}^{\mathrm{Cor},\ell} & \mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\\ \mathrm{J}_{K,21}^{\mathrm{Cor},\ell} & \mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\end{pmatrix}\begin{pmatrix}\mathrm{v}_1\\ \mathrm{v}_2\end{pmatrix}=\begin{pmatrix}\mathrm{v}_1\\ \mathrm{v}_2\end{pmatrix}^\top\mathrm{J}_K^{(\mathrm{Cor},\ell)}\begin{pmatrix}\mathrm{v}_1\\ \mathrm{v}_2\end{pmatrix},\end{aligned}$$

where the matrix $\mathrm{J}_K^{(\mathrm{Cor},\ell)}\in\mathbb{R}^{2K\times2K}$ is given by

$$\mathrm{J}_K^{(\mathrm{Cor},\ell)}:=\begin{pmatrix}\mathrm{J}_{K,11}^{\mathrm{Cor},\ell} & \mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\\ \mathrm{J}_{K,21}^{\mathrm{Cor},\ell} & \mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\end{pmatrix}=\begin{pmatrix}\mathrm{I}_K-\zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)} & \zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\\ \zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)} & \mathrm{I}_K-\zeta^{-1}s_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\end{pmatrix},\quad \ell=1,\ldots,\bar N.$$

Using this argumentation, we conclude that the spectral norm of the two-grid iteration matrix coincides with

$$\|\mathbf{J}_K^{(\mathrm{TG})}\|_2 = \max_{\ell=1,\dots,\bar N+1} \|\mathbf{J}_K^{(\mathrm{TG})}\|_{2,\mathbb{R}^K\otimes \mathrm{w}^{(\ell)}+\mathbb{R}^K\otimes \mathrm{w}^{(N+1-\ell)}} = \max_{\ell=1,\dots,\bar N+1} \|\mathrm{J}_K^{(\mathrm{TG},\ell)}\|_2, \tag{47}$$

where

$$\begin{aligned} \mathrm{J}_K^{(\mathrm{TG},\ell)} &\coloneqq \mathrm{diag}(\mathrm{J}_K^{(\mathrm{Jac},\ell)}, \mathrm{J}_K^{(\mathrm{Jac},N+1-\ell)})^{\nu_1}\mathrm{J}_K^{(\mathrm{Cor},\ell)}\mathrm{diag}(\mathrm{J}_K^{(\mathrm{Jac},\ell)}, \mathrm{J}_K^{(\mathrm{Jac},N+1-\ell)})^{\nu_2}, \quad \ell = 1,\dots,\bar N,\\ \mathrm{J}_K^{(\mathrm{TG},\bar N+1)} &\coloneqq (\mathrm{J}_K^{(\mathrm{Jac},\bar N+1)})^{\nu_1+\nu_2} \end{aligned}$$

while $\mathrm{diag}(\mathrm{J}_K^{(\mathrm{Jac},\ell)}, \mathrm{J}_K^{(\mathrm{Jac},N+1-\ell)}) \in \mathbb{R}^{2K\times 2K}$ is the (block-)diagonal matrix with diagonal entries $\mathrm{J}_K^{(\mathrm{Jac},\ell)}$ and $\mathrm{J}_K^{(\mathrm{Jac},N+1-\ell)}$. Obviously, the spectral norm of $\mathrm{J}_K^{(\mathrm{TG},\bar N+1)}$ satisfies

$$\|\mathrm{J}_K^{(\mathrm{TG},\bar N+1)}\|_2 \leqslant (E^{(\mathrm{Jac},\bar N+1)})^\nu = (1-2\omega_0 s_{\bar N+1}^2)^\nu = (1-\omega_0)^\nu, \tag{48}$$

where $\nu = \nu_1 + \nu_2$ as above. To find upper bounds for the spectral norm of $\mathrm{J}_K^{(\mathrm{TG},\ell)}$ for all $\ell = 1,\dots,\bar N$, we first estimate the spectral norm of the four (block-)submatrices of $\mathrm{J}_K^{(\mathrm{Cor},\ell)}$ and then use Lemma 1.

**Lemma 12.** *The (block-)entries of the auxiliary matrix* $\mathrm{J}_K^{(\mathrm{Cor},\ell)}$ *satisfy*

$$\|\mathrm{J}_{K,11}^{\mathrm{Cor},\ell}\|_2 = \|\mathrm{I}_K - \zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\|_2 \leqslant E_{11}^{(\mathrm{Cor},\ell)} \coloneqq \begin{cases} 1-c_\ell^4 & : \theta \geqslant \frac12 \text{ or } \zeta = \frac12,\\ 1-c_\ell^6 & : \text{otherwise}, \end{cases} \tag{49}$$

$$\|\mathrm{J}_{K,22}^{\mathrm{Cor},\ell}\|_2 = \left\|\mathrm{I}_K - \zeta^{-1}s_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\right\|_2 \leqslant E_{22}^{(\mathrm{Cor},N+1-\ell)} \coloneqq \begin{cases} 1-s_\ell^4 & : \theta \geqslant \frac12 \text{ and } \zeta = 1,\\ 1-s_\ell^6 & : \text{otherwise}, \end{cases} \tag{50}$$

$$\|\mathrm{J}_{K,21}^{\mathrm{Cor},\ell}\|_2 = \left\|\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\right\|_2 \leqslant E_{21}^{(\mathrm{Cor},\ell)} \coloneqq \tfrac{5-2\zeta}{3}s_\ell^2, \tag{51}$$

$$\|\mathrm{J}_{K,12}^{\mathrm{Cor},\ell}\|_2 = \left\|\zeta^{-1}s_\ell^2c_\ell^2(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(N+1-\ell)}\right\|_2 \leqslant E_{12}^{(\mathrm{Cor},N+1-\ell)} \coloneqq c_\ell^2. \tag{52}$$

*for every* $\ell = 1,\dots,\bar N$ *and no matter which (spatial) discretization technique is used.*

*Proof.* The proof of this result can be found in the appendix. □

So far, both components of the two-grid solver, that is, the (block-)Jacobi smoother and the coarse grid correction, are investigated separately by establishing a priori bounds for the error reduction of each spatial Fourier mode. In the next theorem, these estimates will be combined to predict the error reduction in each two-grid iteration with respect to the Euclidean norm.

Strictly speaking, the resulting bound would still depend on the number of spatial grid points $N$ by the definition of $s_\ell^2 \in [0,\frac12]$. To get rid of this implicit dependency, we will exploit the continuous counterpart of $s_\ell = \sin\big(\frac{\pi}{2}\ell(N+1)^{-1}\big)$ for $\ell = 1,\dots,N$ which reads $s_\iota = \sin(\frac{\pi}{2}\iota)$ for $\iota \in [0,1]$ without becoming ambiguous. In what follows, this notational convention will also be used for quantities like $E^{(\mathrm{Jac},\cdot)}$ and $E_{jk}^{(\mathrm{Cor},\cdot)}$.

**Theorem 13.** *The spectral norm of the two-grid iteration matrix is bounded from above by*

$$\|\mathbf{J}_K^{(\mathrm{TG})}\|_2 \leqslant E^{(\mathrm{TG})} \coloneqq \max_{\iota\in[0,\frac12]} E^{(\mathrm{TG},\iota)}, \tag{53}$$

*where*

$$E^{(\mathrm{TG},\iota)} \coloneqq \left\| \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_1} \begin{pmatrix} E_{11}^{(\mathrm{Cor},\iota)} & E_{12}^{(\mathrm{Cor},1-\iota)} \\ E_{21}^{(\mathrm{Cor},\iota)} & E_{22}^{(\mathrm{Cor},1-\iota)} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_2} \right\|_2, \quad \iota \in [0,\tfrac12]. \tag{54}$$

*Proof.* Employing Lemma 1, Theorem 8, and Lemma 12, it can be easily verified that

$$\|\mathrm{J}_K^{(\mathrm{TG},\ell)}\|_2 \leqslant E_2^{(\mathrm{TG},\ell/(N+1))}, \quad \ell = 1,\dots\bar N.$$

Furthermore, the inequality $\|\mathrm{J}_K^{(\mathrm{TG},\bar{N}+1)}\|_2 \leqslant E_2^{(\mathrm{TG},\frac{1}{2})}$ is valid because

$$\begin{aligned}
E^{(\mathrm{TG},\frac{1}{2})} &= \left\| \begin{pmatrix} E^{(\mathrm{Jac},\frac{1}{2})} & \\ & E^{(\mathrm{Jac},\frac{1}{2})} \end{pmatrix}^{\nu_1} \begin{pmatrix} E_{11}^{(\mathrm{Cor},\frac{1}{2})} & E_{12}^{(\mathrm{Cor},\frac{1}{2})} \\ E_{21}^{(\mathrm{Cor},\frac{1}{2})} & E_{22}^{(\mathrm{Cor},\frac{1}{2})} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\frac{1}{2})} & \\ & E^{(\mathrm{Jac},\frac{1}{2})} \end{pmatrix}^{\nu_2} \right\|_2 \\
&= (E^{(\mathrm{Jac},\frac{1}{2})})^{\nu} \left\| \begin{pmatrix} E_{11}^{(\mathrm{Cor},\frac{1}{2})} & E_{12}^{(\mathrm{Cor},\frac{1}{2})} \\ E_{21}^{(\mathrm{Cor},\frac{1}{2})} & E_{22}^{(\mathrm{Cor},\frac{1}{2})} \end{pmatrix} \right\|_2 \\
&\geqslant (E^{(\mathrm{Jac},\frac{1}{2})})^{\nu} \left\| \begin{pmatrix} E_{11}^{(\mathrm{Cor},\frac{1}{2})} & E_{12}^{(\mathrm{Cor},\frac{1}{2})} \\ E_{21}^{(\mathrm{Cor},\frac{1}{2})} & E_{22}^{(\mathrm{Cor},\frac{1}{2})} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\|_2 \left\| \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\|_2^{-1} = (E^{(\mathrm{Jac},\frac{1}{2})})^{\nu} \frac{\sqrt{2}}{2} \left\| \begin{pmatrix} E_{11}^{(\mathrm{Cor},\frac{1}{2})} + E_{12}^{(\mathrm{Cor},\frac{1}{2})} \\ E_{21}^{(\mathrm{Cor},\frac{1}{2})} + E_{22}^{(\mathrm{Cor},\frac{1}{2})} \end{pmatrix} \right\|_2 \\
&\geqslant (E^{(\mathrm{Jac},\frac{1}{2})})^{\nu} \frac{\sqrt{2}}{2} \sqrt{(1 - \tfrac{1}{4} + \tfrac{1}{2})^2 + (1 - \tfrac{1}{4} + \tfrac{1}{2})^2} = \tfrac{5}{4} (E^{(\mathrm{Jac},\frac{1}{2})})^{\nu} \geqslant \tfrac{5}{4} \|\mathrm{J}_K^{(\mathrm{TG},\bar{N}+1)}\|_2
\end{aligned}$$

by (48). Then the statement of the theorem follows by (47). □

The above theorem states that the spectral norm of the two-grid iteration matrix can be bounded from above by taking the maximum over the spectral norm of certain $2 \times 2$-matrices. These matrices do not depend on the number of spatial grid points or the total size of blocked time steps any more resulting in a rate of convergence which might only depend on the CFL number $\lambda = \tau h^{-2}$. In what follows, we will see that the spectral norm of the two-grid iteration matrix is even uniformly bounded from above independently of $\lambda$ for some practically relevant configurations.

**Corollary 14.** *In case of finite differences and $\theta \geqslant \frac{1}{2}$, the two-grid method using the relaxation parameter $\omega = \omega_0 = \frac{2}{3}$ converges monotonically if $\nu_2 \geqslant 1$ and*

$$\|\mathbf{J}_K^{(\mathrm{TG})}\|_2 \leqslant \hat{E}^{(\mathrm{TG})} := \sqrt{\tfrac{45}{16}(1+\nu_2)^{-2}(\tfrac{\nu_2}{1+\nu_2})^{2\nu_2} + 2 \cdot 3^{-2\nu_2}} < 1. \tag{55}$$

*Proof.* For $\iota \in [0, \frac{1}{2}]$, we have

$$\begin{aligned}
(E^{(\mathrm{TG},\iota)})^2 &= \left\| \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_1} \begin{pmatrix} E_{11}^{(\mathrm{Cor},\iota)} & E_{12}^{(\mathrm{Cor},1-\iota)} \\ E_{21}^{(\mathrm{Cor},\iota)} & E_{22}^{(\mathrm{Cor},1-\iota)} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_2} \right\|_2^2 \\
&\leqslant \underbrace{\left\| \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix} \right\|_2^{2\nu_1}}_{\leqslant 1 \text{ by Theorem 8}} \left\| \begin{pmatrix} E_{11}^{(\mathrm{Cor},\iota)} & E_{12}^{(\mathrm{Cor},1-\iota)} \\ E_{21}^{(\mathrm{Cor},\iota)} & E_{22}^{(\mathrm{Cor},1-\iota)} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_2} \right\|_{\mathrm{F}}^2 \\
&\leqslant \left(E^{(\mathrm{Jac},\iota)}\right)^{2\nu_2} \left( \left(E_{11}^{(\mathrm{Cor},\iota)}\right)^2 + \left(E_{21}^{(\mathrm{Cor},\iota)}\right)^2 \right) + \left(E^{(\mathrm{Jac},1-\iota)}\right)^{2\nu_2} \left( \left(E_{12}^{(\mathrm{Cor},1-\iota)}\right)^2 + \left(E_{22}^{(\mathrm{Cor},1-\iota)}\right)^2 \right) \\
&= \left(1 - \tfrac{4}{3} s_\iota^2\right)^{2\nu_2} \left((1 - c_\iota^4)^2 + s_\iota^4\right) + 3^{-2\nu_2} \left((1 - s_\iota^4)^2 + c_\iota^4\right) \\
&\leqslant \left(1 - \tfrac{4}{3} s_\iota^2\right)^{2\nu_2} \left((1 - c_\iota^4)^2 + s_\iota^4\right) + 2 \cdot 3^{-2\nu_2} \\
&= s_\iota^4 (1 - \tfrac{4}{3} s_\iota^2)^{2\nu_2} \left(5 - 3 s_\iota^2 - s_\iota^2 (1 - s_\iota^2)\right) + 2 \cdot 3^{-2\nu_2} \\
&\leqslant 5 \tfrac{9}{16} (1 + \nu_2)^{-2} (\tfrac{\nu_2}{1+\nu_2})^{2\nu_2} + 2 \cdot 3^{-2\nu_2} = (\hat{E}^{(\mathrm{TG})})^2,
\end{aligned}$$

because $s_\iota^2 (1 - \frac{4}{3} s_\iota^2)^{\nu_2}$ attains its maximum at $s_\iota^2 = \frac{3}{4}(1+\nu_2)^{-1} \in (0, \frac{1}{2})$. Finally, the bound $\hat{E}^{(\mathrm{TG})}$ is smaller than 1 due to the fact that

$$\begin{aligned}
(\hat{E}^{(\mathrm{TG})})^2 &= \tfrac{45}{16} (1+\nu_2)^{-2} (\tfrac{\nu_2}{1+\nu_2})^{2\nu_2} + 2 \cdot 3^{-2\nu_2} \\
&\leqslant \tfrac{45}{16} (1+\nu_2)^{-2} (\tfrac{\nu_2}{1+\nu_2})^{2} + 2 \cdot 3^{-2} \leqslant \tfrac{45}{16} (\tfrac{\nu_2}{2\nu_2 + \nu_2^2})^2 + 2 \cdot 3^{-2} \leqslant \tfrac{45}{16} (\tfrac{1}{3})^2 + 2 \cdot 3^{-2} = \tfrac{77}{144}.
\end{aligned}$$

□

**Corollary 15.** *In case of a finite element approximation and $\theta = \frac{1}{2}$, the two-grid method using the relaxation parameter $\omega = \omega_0 = \frac{4}{5}$ converges monotonically if $\nu_2 \geqslant 1$ and*

$$\|\mathbf{J}_K^{(\mathrm{TG})}\|_2 \leqslant \hat{E}^{(\mathrm{TG})} := \sqrt{\tfrac{325}{144}(1+\nu_2)^{-2}(\tfrac{\nu_2}{1+\nu_2})^{2\nu_2} + 2(\tfrac{3}{5})^{2\nu_2}} < 1. \tag{56}$$

*Proof.* For $\iota \in [0, \frac{1}{2}]$, we have

$$\begin{aligned}
(E^{(\mathrm{TG},\iota)})^2 &= \left\| \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_1} \begin{pmatrix} E_{11}^{(\mathrm{Cor},\iota)} & E_{12}^{(\mathrm{Cor},1-\iota)} \\ E_{21}^{(\mathrm{Cor},\iota)} & E_{22}^{(\mathrm{Cor},1-\iota)} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_2} \right\|_2^2 \\
&\leqslant \underbrace{\left\| \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix} \right\|_2^{2\nu_1}}_{\leqslant 1 \text{ by Theorem 8}} \left\| \begin{pmatrix} E_{11}^{(\mathrm{Cor},\iota)} & E_{12}^{(\mathrm{Cor},1-\iota)} \\ E_{21}^{(\mathrm{Cor},\iota)} & E_{22}^{(\mathrm{Cor},1-\iota)} \end{pmatrix} \begin{pmatrix} E^{(\mathrm{Jac},\iota)} & \\ & E^{(\mathrm{Jac},1-\iota)} \end{pmatrix}^{\nu_2} \right\|_{\mathrm{F}}^2 \\
&\leqslant \left(E^{(\mathrm{Jac},\iota)}\right)^{2\nu_2} \left( \left(E_{11}^{(\mathrm{Cor},\iota)}\right)^2 + \left(E_{21}^{(\mathrm{Cor},\iota)}\right)^2 \right) + \left(E^{(\mathrm{Jac},1-\iota)}\right)^{2\nu_2} \left( \left(E_{12}^{(\mathrm{Cor},1-\iota)}\right)^2 + \left(E_{22}^{(\mathrm{Cor},1-\iota)}\right)^2 \right) \\
&= \left(1 - \tfrac{8}{5} s_\iota^2\right)^{2\nu_2} \left((1 - c_\iota^4)^2 + \tfrac{16}{9} s_\iota^4\right) + \left(\tfrac{3}{5}\right)^{2\nu_2} \left((1 - s_\iota^6)^2 + c_\iota^4\right) \\
&\leqslant \left(1 - \tfrac{8}{5} s_\iota^2\right)^{2\nu_2} \left((1 - c_\iota^4)^2 + \tfrac{16}{9} s_\iota^4\right) + 2\left(\tfrac{3}{5}\right)^{2\nu_2} \\
&= s_\iota^4 \left(1 - \tfrac{8}{5} s_\iota^2\right)^{2\nu_2} \left(4 - 3s_\iota^2 - s_\iota^2(1 - s_\iota^2) + \tfrac{16}{9}\right) + 2\left(\tfrac{3}{5}\right)^{2\nu_2} \\
&\leqslant \tfrac{52}{9} \tfrac{25}{64} (1 + \nu_2)^{-2} \left(\tfrac{\nu_2}{1+\nu_2}\right)^{2\nu_2} + 2\left(\tfrac{3}{5}\right)^{2\nu_2} = (\hat{E}^{(\mathrm{TG})})^2,
\end{aligned}$$

because $s_\iota^2(1 - \frac{8}{5} s_\iota^2)^{\nu_2}$ attains its maximum at $s_\iota^2 = \frac{5}{8}(1 + \nu_2)^{-1} \in (0, \frac{1}{2})$. Finally, the bound $\hat{E}^{(\mathrm{TG})}$ is smaller than 1 due to the fact that

$$\begin{aligned}
(\hat{E}^{(\mathrm{TG})})^2 &= \tfrac{325}{144} (1 + \nu_2)^{-2} \left(\tfrac{\nu_2}{1+\nu_2}\right)^{2\nu_2} + 2\left(\tfrac{3}{5}\right)^{2\nu_2} \\
&\leqslant \tfrac{325}{144} (1 + \nu_2)^{-2} \left(\tfrac{\nu_2}{1+\nu_2}\right)^2 + 2\left(\tfrac{3}{5}\right)^2 \leqslant \tfrac{325}{144} \left(\tfrac{\nu_2}{2\nu_2+\nu_2^2}\right)^2 + 2\left(\tfrac{3}{5}\right)^2 \leqslant \tfrac{325}{144} \left(\tfrac{1}{3}\right)^2 + 2\left(\tfrac{3}{5}\right)^2 = \tfrac{2491}{2566}. \qquad \square
\end{aligned}$$

Similarly, bounds can also be derived for $\theta \geqslant \frac{1}{2}$ in case of a finite element approximation and/or by considering pre-smoothing, too.

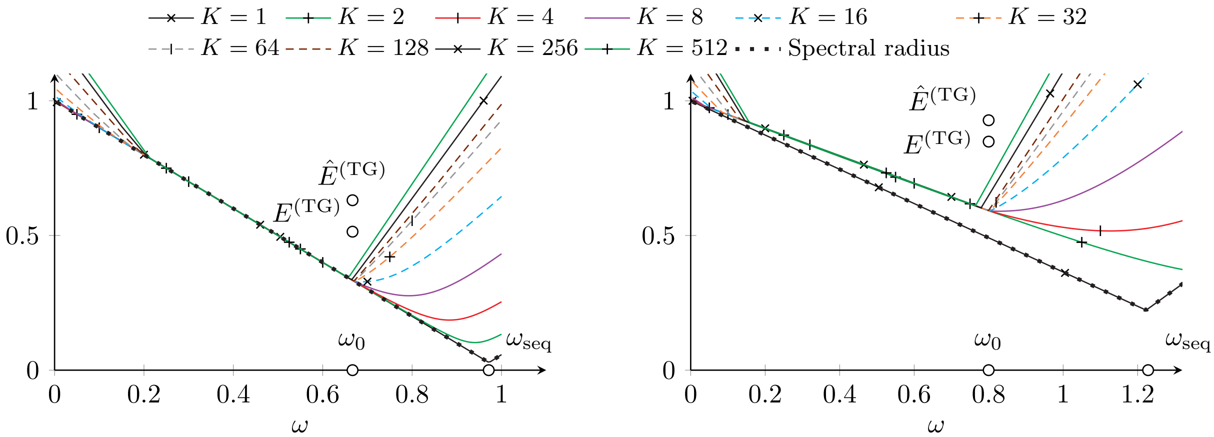
## 6.4 Discussion on (optimal) convergence behavior

When it comes to the convergence analysis of iterative solution strategies, it is common practice to study the *asymptotic* rate of convergence. For linear methods, this quantity coincides with the spectral radius of the iteration matrix and, unfortunately, only approximates the defect reduction after a sufficient number of iterations. In particular, there is no control over the solution behavior during the first few iterations and, hence, a priori predictions of the computational cost required to gain a certain number of digits in accuracy is impossible. For error estimates with respect to a specific vector norm, the corresponding induced matrix norm of the iteration matrix has to be considered. Thus, the optimal choice of involved parameters may highly depend on the (matrix) norm under investigation.

For instance, the discrepancy between the spectral norm and the spectral radius of the two-grid iteration matrix caused by different damping parameters of the (block-)Jacobi smoother is illustrated in Fig. 2 for a single post-smoothing step. The choice of $\omega_{\mathrm{seq}}$ seems to be a very good approximation of the optimal relaxation parameter to minimize the spectral radius, no matter how many time steps $K$ are blocked. While there is hardly any difference between the spectral radius and the spectral norm for $K = 1$, that is, a sequential computation, the latter quantity grows monotonically if $K$ increases and $\omega$ is chosen too large. On the other hand, relaxation of the (block-)Jacobi update using $\omega_0$ results in adequate convergence rates for all considered values of $K$. Furthermore, the spectral radius and spectral norm of the two-grid iteration matrix are close to each other for this configuration, or even nearly coincide in case of a finite difference approximation. Therefore, a uniform and monotone convergence of the solution iterates can be expected and a rapid error reduction starting from the beginning is guaranteed.

The practical impact of this behavior can be observed in Fig. 3 illustrating the history of the Euclidean norm of the residual for the two-grid solver corresponding to (11). Here, the initial guess is given by $\mathbf{u}^{(0)} = \mathbf{0}$ and the discrete initial data reads

$$\mathrm{u}_i^{(0)} = \begin{cases} 1 & : |x_i - \frac{1}{2}| < \frac{1}{5}, \\ 0 & : |x_i - \frac{1}{2}| \geqslant \frac{1}{5}. \end{cases}$$




(a) Finite differences.

(b) Finite elements.

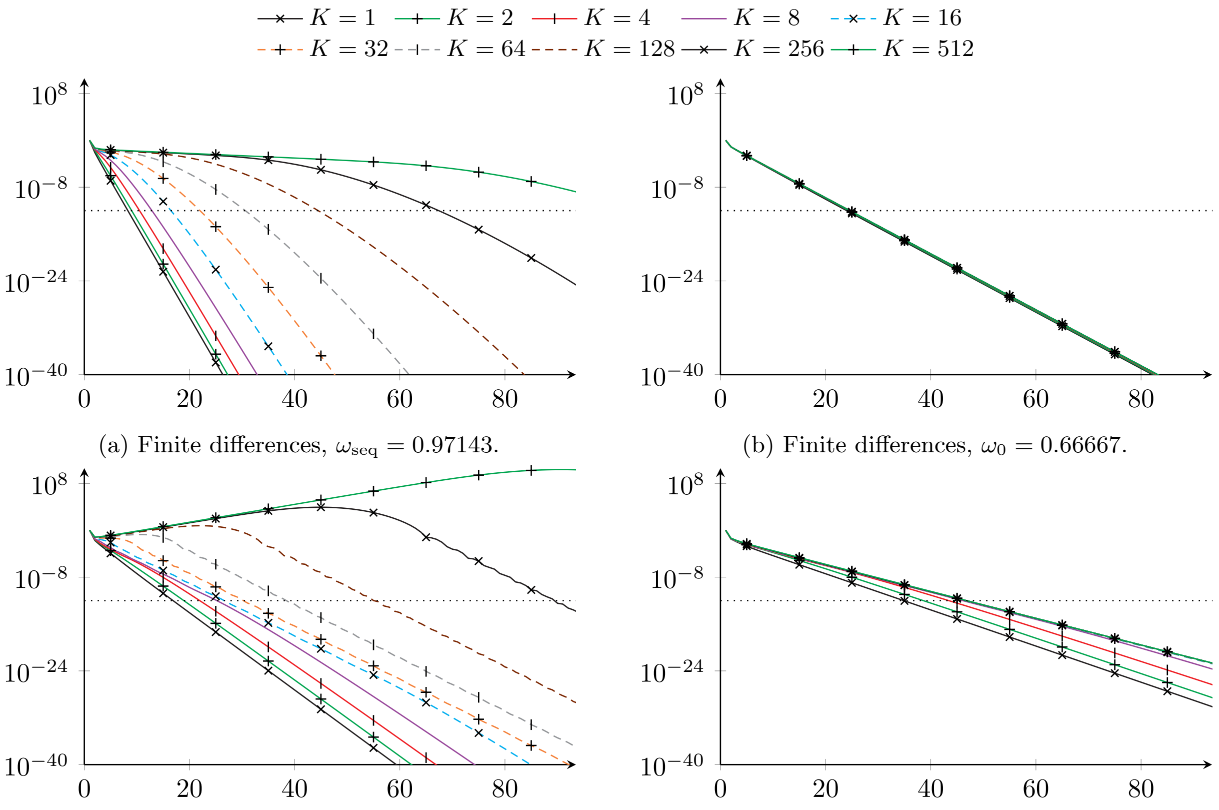
Figure 2: Spectral norm (and spectral radius) of two-grid iteration matrix depending on relaxation parameter $\omega \in (0, 1]$ for $\nu_1 = 0$, $\nu_2 = 1$, $\theta = \frac{1}{2}$, $h = 2^{-4}$, $\tau = 2^{-12}$.

When $\omega_{\mathrm{seq}}$ is used to relax the (block-)Jacobi smoother, a uniformly bounded defect reduction cannot be guaranteed and the Euclidean norm of the residual might even grow initially if the number of blocked time steps $K$ is too large for a finite element discretization. In contrast to this, the iterates of the two-grid solver using the damping parameter $\omega_0$ converge monotonically to the exact solution so that a certain tolerance, like $10^{-12}$, may be reached with less computational effort although the asymptotic rate of convergence deteriorates.

## 7 Conclusion

In this work, the convergence of a time-simultaneous two-grid solver for the one-dimensional heat equation discretized in space by finite differences or finite elements and integrated in time using the $\theta$-scheme is analyzed. Although the dimension of the all-at-once system grows arbitrarily as the number of blocked time steps increases, the corresponding condition number is bounded from above by a constant which only depends on parameters of the underlying sequential discretization technique. The proof of this statement highly exploits a tensor product approach and a spatial Fourier analysis. Both techniques also provide the possibility to investigate the convergence behavior of the considered two-grid solver. For a specific choice of the relaxation parameter used by the (block-)Jacobi smoother, explicitly determined bounds for the spectral norm of the iteration matrix predict a convergence rate which is uniformly bounded no matter how many time steps are treated simultaneously. Therefore, solution of the all-at-once system just requires computational costs which are linear with respect to the *global* number of degrees of freedom and blocking more time steps does not arbitrarily increase the overall complexity.

Caused by these generalizations and simplifications, the estimates proposed in this work cannot reflect the improved convergence behavior for very small time increments and/or number of blocked time steps. Therefore, further efforts have to be invested in achieving more accurate estimates for the convergence rate in the limit of vanishing time increments. Such results might be beneficial to understand and further improve solution algorithms which might also exploit temporal coarsening strategies as proposed in [Fra+18; HV95]. Furthermore, extension of the presented results to higher dimensions and more complex geometries might be of interest to enlarge the practical relevancy.




(a) Finite differences, $\omega_{\text{seq}} = 0.97143$.

(b) Finite differences, $\omega_0 = 0.66667$.

(c) Finite elements, $\omega_{\text{seq}} = 1.22807$.

(d) Finite elements, $\omega_0 = 0.8$.

Figure 3: History of relative norm of residual, $\theta = \frac{1}{2}$, $\nu_1 = 0$, $\nu_2 = 1$, $h = 2^{-4}$, $\tau = 2^{-12}$.

## References


[BH01] S. Börm and R. Hiptmair. "Analysis of tensor product multigrid". In: *Numerical Algorithms* 26 (3 2001), pp. 219–234.

[Bra76] Achi Brandt. *Multi-level Adaptive Techniques (mlat), 1; the Multi-grid Method.* IBM Thomas J. Watson Research Division, 1976.

[Dün+19] J. Dünnebacke et al. *A time–simultaneous multigrid method for parabolic evolution equations.* Tech. rep. Ergebnisberichte des Instituts für Angewandte Mathematik, Nummer 619. Fakultät für Mathematik, TU Dortmund (accepted in Numerical Mathematics and Advanced Applications ENUMATH 2019). Dec. 2019.

[Dün+21] Jonas Dünnebacke et al. "Increased space-parallelism via time-simultaneous Newton-multigrid methods for nonstationary nonlinear PDE problems". In: *The International Journal of High Performance Computing Applications* (2021). URL: `https://doi.org/10.1177/10943420211001940`.

[EM12] Matthew Emmett and Michael Minion. "Toward an efficient parallel in time method for partial differential equations". In: *Communications in Applied Mathematics and Computational Science* 7.1 (2012), pp. 105–132. URL: `https://doi.org/10.2140/camcos.2012.7.105`.

[Fal+17a] R. D. Falgout et al. "Multigrid methods with space–time concurrency". In: *Computing and Visualization in Science* 18 (4 2017), pp. 123–143. URL: `https://doi.org/10.1007/s00791-017-0283-9`.

[Fal+17b] R. D. Falgout et al. "Multigrid Reduction in Time for Nonlinear Parabolic Problems: A Case Study". In: *SIAM Journal on Scientific Computing* 39.5 (2017), S298–S322. URL: `https://doi.org/10.1137/16M1082330`.

[Fra+18] Sebastião Romero Franco et al. "Multigrid method based on a space-time approach with standard coarsening for parabolic problems". In: *Applied Mathematics and Computation* 317 (2018), pp. 25–34. URL: `http://www.sciencedirect.com/science/article/pii/S0096300317305945`.

[Gan15] Martin J. Gander. "50 Years of Time Parallel Time Integration". In: *Multiple Shooting and Time Domain Decomposition Methods.* Ed. by Thomas Carraro et al. Cham: Springer International Publishing, 2015, pp. 69–113.

[Ger31] S. A. Gershgorin. "Über die Abgrenzung der Eigenwerte einer Matrix". German. In: *Bull. Acad. Sci. URSS* 1931.6 (1931), pp. 749–754.

[GK02] Eldar Giladi and Herbert B. Keller. "Space-time domain decomposition for parabolic problems". In: *Numerische Mathematik* 93 (2 2002), pp. 279–313. URL: `https://doi.org/10.1007/s002110100345`.

[GN16] Martin J. Gander and Martin Neumüller. "Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems". In: *SIAM Journal on Scientific Computing* 38.4 (2016), A2173–A2208. URL: `https://doi.org/10.1137/15M1046605`.

[GS58] Ulf Grenander and Gabor Szegö. *Toeplitz forms and their applications.* Univ of California Press, 1958.

[GS98] Martin J. Gander and Andrew M. Stuart. "Space-Time Continuous Analysis of Waveform Relaxation for the Heat Equation". In: *SIAM Journal on Scientific Computing* 19.6 (1998), pp. 2014–2031. URL: `https://doi.org/10.1137/S1064827596305337`.

[Hac13] Wolfgang Hackbusch. *Multi-grid methods and applications.* Vol. 4. Springer Science & Business Media, 2013.

[Hac85] Wolfgang Hackbusch. "Parabolic Multi-Grid Methods". In: *Proc. of the Sixth Int'l. Symposium on Computing Methods in Applied Sciences and Engineering, VI.* Versailles, France: North-Holland Publishing Co., 1985, pp. 189–197.

[Hes+20] Andreas Hessenthaler et al. “Multilevel Convergence Analysis of Multigrid-Reduction-in-Time”. In: *SIAM Journal on Scientific Computing* 42.2 (2020), A771–A796. URL: https://doi.org/10.1137/19M1238812.

[HV95] G. Horton and S. Vandewalle. “A Space-Time Multigrid Method for Parabolic Partial Differential Equations”. In: *SIAM Journal on Scientific Computing* 16.4 (1995), pp. 848–864. URL: https://doi.org/10.1137/0916050.

[HVW95] G. Horton, S. Vandewalle, and P. Worley. “An Algorithm with Polylog Parallel Complexity for Solving Parabolic Partial Differential Equations”. In: *SIAM Journal on Scientific Computing* 16.3 (1995), pp. 531–541. URL: https://doi.org/10.1137/0916034.

[JV96] Jan Janssen and Stefan Vandewalle. “Multigrid Waveform Relaxation on Spatial Finite Element Meshes: The Discrete-Time Case”. In: *SIAM Journal on Scientific Computing* 17.1 (1996), pp. 133–155. URL: https://doi.org/10.1137/0917011.

[LMT01] Jacques-Louis Lions, Yvon Maday, and Gabriel Turinici. “Résolution d’EDP par un schéma en temps «pararéel »”. In: *Comptes Rendus de l’Académie des Sciences - Series I - Mathematics* 332.7 (2001), pp. 661–668. URL: http://www.sciencedirect.com/science/article/pii/S0764444200017936.

[LO87] Ch. Lubich and A. Ostermann. “Multi-grid dynamic iteration for parabolic equations”. In: *BIT Numerical Mathematics* 27 (2 1987), pp. 216–234. URL: https://doi.org/10.1007/BF01934186.

[LRS82] E. Lelarasmee, A. E. Ruehli, and A. L. Sangiovanni-Vincentelli. “The Waveform Relaxation Method for Time-Domain Analysis of Large Scale Integrated Circuits”. In: *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems* 1.3 (1982), pp. 131–145.

[Min10] Michael Minion. “A hybrid parareal spectral deferred corrections method”. In: *Communications in Applied Mathematics and Computational Science* 5.2 (2010), pp. 265–301. URL: https://doi.org/10.2140/camcos.2010.5.265.

[OS20] Benjamin W. Ong and Jacob B. Schroder. “Applications of time parallelization”. In: *Computing and Visualization in Science* 23 (1 2020). URL: https://doi.org/10.1007/s00791-020-00331-4.

[Reu02] Arnold Reusken. “Convergence analysis of a multigrid method for convection–diffusion equations”. In: *Numerische Mathematik* 91 (2 2002). URL: https://doi.org/10.1007/s002110100312.

[Tar90] Pablo Tarazaga. “Eigenvalue estimates for symmetric matrices”. In: *Linear Algebra and its Applications* 135 (1990), pp. 171–179. URL: http://www.sciencedirect.com/science/article/pii/0024379590901202.

[Tre10] WF Trench. *Spectral decomposition of Kac–Murdock–Szegő matrices. The Selected Works of William F. Trench.* 2010.

[VH95] S. Vandewalle and G. Horton. “Fourier mode analysis of the multigrid waveform relaxation and time-parallel multigrid methods”. In: 54 (4 1995), pp. 317–330.


# A Appendix

To prove the statement of Theorem 3, some preliminary results have to be summarized.

**Lemma 16.** *The eigenvalues of the Kac-Murdock-Szegö matrix* $\mathrm{E}(\rho) = (\rho^{|i-j|})_{i,j=1}^{M}$, $M \geqslant 2$, *for* $\rho \in (0,1)$ *are given by [GS58]*

$$\lambda_k(\rho) = \frac{1-\rho^2}{1-2\rho\cos(\gamma_k)+\rho^2}, \quad k = 1, \dots, M, \tag{57}$$

*where* $\gamma_1, \dots, \gamma_M \in (0, \pi)$ *are the roots of*

$$f(\gamma) = \sin\big((M+1)\gamma\big) - 2\rho\sin(M\gamma) + \rho^2\sin\big((M-1)\gamma\big) \tag{58}$$

*and can be estimated by [Tre10]*

$$\frac{(k-1)\pi}{M} < \gamma_k < \frac{k\pi}{M+1}, \quad k = 1, \ldots, M.$$

*Therefore, the spectrum of* $\mathrm{E}(\rho)$ *satisfies*

$$\sigma\big(\mathrm{E}(\rho)\big) \subset \Big(\frac{1-\rho}{1+\rho}, \frac{1+\rho}{1-\rho}\Big). \tag{59}$$

**Corollary 17.** *The Kac-Murdock-Szegö matrix* $\mathrm{E}(\rho)$ *is similar to* $\mathrm{E}(-\rho)$ *and, hence, both matrices have the same eigenvalues.*

**Lemma 18.** *The Hankel matrix* $\mathrm{E}(\rho) = (\rho^{2M-i-j})_{i,j=1}^{M}$, $M \in \mathbb{N}$, *for* $\rho \in \mathbb{R}$ *is positive semidefinite and the only non-vanishing eigenvalue is given by its trace while the corresponding eigenvector reads* $(\rho^{M-1}, \rho^{M-2}, \ldots, \rho^0)^\top$.

*Proof.* The statement of this lemma can be easily verified and, hence, will be omitted. □

Based on these results, Theorem 3 can be shown by some algebraic manipulations.

*Proof of Theorem 3.* First of all, let us consider the special case $f_2 = 0$. Then the matrix $\mathrm{F}^{-1}\mathrm{E}$ coincides with $f_1^{-1}\mathrm{E}$, which is well defined because $f_1$ does not vanish by assumption of the theorem. Therefore, we have

$$(\mathrm{F}^{-1}\mathrm{E})^\top \mathrm{F}^{-1}\mathrm{E} = f_1^{-2}\begin{pmatrix} e_1^2+e_2^2 & e_1e_2 & & \\ e_1e_2 & \ddots & \ddots & \\ & \ddots & e_1^2+e_2^2 & e_1e_2 \\ & & e_1e_2 & e_1^2 \end{pmatrix}.$$

Obviously, this matrix is positive semidefinite while the maximal eigenvalue is bounded from above by $e_1^2 + e_2^2 + 2|e_1e_2|$ according to the Gershgorin circle theorem [Ger31]. Then the statement of the theorem directly follows by distinguishing between $e_1e_2 \geqslant 0$ and $e_1e_2 < 0$.

If $f_2 \neq 0$, we first note that the inverse of F reads

$$\mathrm{F}^{-1} = \begin{pmatrix} f_1^{-1} & & & \\ (-f_1^{-1}f_2)f_1^{-1} & f_1^{-1} & & \\ \vdots & \ddots & \ddots & \\ (-f_1^{-1}f_2)^{M-1}f_1^{-1} & \cdots & -(f_1^{-1}f_2)f_1^{-1} & f_1^{-1} \end{pmatrix}$$

and, hence,

$$\begin{aligned} \mathrm{F}^{-1}\mathrm{E} &= \begin{pmatrix} f_1^{-1} & & & \\ (-f_1^{-1}f_2)f_1^{-1} & f_1^{-1} & & \\ \vdots & \ddots & \ddots & \\ (-f_1^{-1}f_2)^{M-1}f_1^{-1} & \cdots & -(f_1^{-1}f_2)f_1^{-1} & f_1^{-1} \end{pmatrix} \begin{pmatrix} e_1 & & & \\ e_2 & e_1 & & \\ & \ddots & \ddots & \\ & & e_2 & e_1 \end{pmatrix} \\ &= \begin{pmatrix} f_1^{-1}e_1 & & & \\ f_1^{-1}(e_2 - f_2f_1^{-1}e_1) & f_1^{-1}e_1 & & \\ \vdots & \ddots & \ddots & \\ (-f_1^{-1}f_2)^{M-2}f_1^{-1}(e_2 - f_2f_1^{-1}e_1) & \cdots & f_1^{-1}(e_2 - f_2f_1^{-1}e_1) & f_1^{-1}e_1 \end{pmatrix} \\ &= \begin{pmatrix} s_1 & & & \\ s_3 & s_1 & & \\ \vdots & \ddots & \ddots & \\ s_2^{M-2}s_3 & \cdots & s_3 & s_1 \end{pmatrix}, \end{aligned}$$

where $s_1 = f_1^{-1} e_1$, $s_2 = -f_1^{-1} f_2 \in (-1,1)$, $s_3 = f_1^{-1}(e_2 - f_2 f_1^{-1} e_1)$. Therefore, the symmetric and positive semidefinite matrix $\mathrm{T} = (\mathrm{F}^{-1}\mathrm{E})^\top \mathrm{F}^{-1}\mathrm{E}$ possesses the entries

$$\begin{aligned}
t_{ii} &= s_1 \cdot s_1 + s_3 \cdot s_3 + \ldots + s_3 s_2^{M-1-i} \cdot s_2^{M-1-i} s_3 \\
&= s_1^2 + s_3 \Big( \sum_{j=0}^{M-1-i} s_2^{2j} \Big) s_3 = s_1^2 + s_3^2 \frac{1 - s_2^{2M-2i}}{1 - s_2^2}, && i = 1, \ldots, M, \\
t_{ij} &= s_1 \cdot s_2^{i-j-1} s_3 + s_3 \cdot s_2^{i-j} s_3 + s_3 s_2 \cdot s_2^{i-j+1} s_3 + \ldots + s_3 s_2^{M-1-i} \cdot s_2^{M-1-j} s_3 \\
&= s_1 s_2^{i-j-1} s_3 + s_3 \Big( \sum_{l=0}^{M-1-i} s_2^{2l} \Big) s_2^{i-j} s_3 \\
&= s_1 s_3 s_2^{i-j-1} + s_3^2 \frac{1 - s_2^{2M-2i}}{1 - s_2^2} s_2^{i-j} = t_{ji}, && i = 1, \ldots, M, \quad j = 1, \ldots, i-1.
\end{aligned}$$

To estimate the largest eigenvalue of T, the matrix can be decomposed into

$$\begin{aligned}
\mathrm{T} &= \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3, \\
\mathrm{T}_1 &= \begin{pmatrix} s_1^2 + \frac{s_3^2}{1-s_2^2} - p & & \\ & \ddots & \\ & & s_1^2 + \frac{s_3^2}{1-s_2^2} - p \end{pmatrix} = \Big( s_1^2 + \frac{s_3^2}{1 - s_2^2} - p \Big) \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{pmatrix}, \\
\mathrm{T}_2 &= \begin{pmatrix} p & s_1 s_3 + \frac{s_3^2}{1-s_2^2} s_2 & \cdots & s_1 s_3 s_2^{M-2} + \frac{s_3^2}{1-s_2^2} s_2^{M-1} \\ s_1 s_3 + \frac{s_3^2}{1-s_2^2} s_2 & \ddots & & \vdots \\ \vdots & & \ddots & s_1 s_3 + \frac{s_3^2}{1-s_2^2} s_2 \\ s_1 s_3 s_2^{M-2} + \frac{s_3^2}{1-s_2^2} s_2^{M-1} & \cdots & s_1 s_3 + \frac{s_3^2}{1-s_2^2} s_2 & p \end{pmatrix} \\
&= p \begin{pmatrix} s_2^0 & s_2^1 & \cdots & s_2^{M-1} \\ s_2^1 & \ddots & & \vdots \\ \vdots & & \ddots & s_2^1 \\ s_2^{M-1} & \cdots & s_2^1 & s_2^0 \end{pmatrix}, \\
\mathrm{T}_3 &= \frac{-s_3^2}{1 - s_2^2} \begin{pmatrix} s_2^{2M-1-1} & s_2^{2M-1-2} & \cdots & s_2^{2M-1-M} \\ s_2^{2M-2-1} & \ddots & & \vdots \\ \vdots & & \ddots & s_2^{2M-(M-1)-M} \\ s_2^{2M-M-1} & \cdots & s_2^{2M-M-(M-1)} & s_2^{2M-M-M} \end{pmatrix}
\end{aligned}$$

where

$$\begin{aligned}
p &:= s_1 s_3 s_2^{-1} + \frac{s_3^2}{1 - s_2^2} = s_3 \frac{s_1 - s_1 s_2^2 + s_2 s_3}{s_2 (1 - s_2^2)} \\
&= f_1^{-1}(e_2 - f_1^{-1} f_2 e_1) \frac{f_1^{-1} e_1 - f_1^{-1} e_1 f_1^{-2} f_2^2 - f_1^{-1} f_2 f_1^{-1}(e_2 - f_1^{-1} f_2 e_1)}{-f_1^{-1} f_2 (1 - f_1^{-2} f_2^2)} \\
&= (f_1 e_2 - f_2 e_1) \frac{f_1 e_1 - f_1^{-1} f_2^2 e_1 - f_2 (e_2 - f_1^{-1} f_2 e_1)}{f_1 f_2 (f_2^2 - f_1^2)} \\
&= (f_1 e_2 - f_2 e_1) \frac{f_1 e_1 - f_2 e_2}{f_1 f_2 (f_2^2 - f_1^2)} = \frac{\eta}{f_1 f_2 (f_2^2 - f_1^2)}.
\end{aligned}$$

Obviously, the maximal eigenvalue of $\mathrm{T}_3$ is bounded from above by zero according to Lemma 18 and the fact that $s_2^2 < 1$. By Corollary 17, the spectrum of $\mathrm{T}_2$ satisfies

$$\sigma(\mathrm{T}_2) \subseteq \begin{cases} \left[p\frac{1-s_2}{1+s_2}, p\frac{1+s_2}{1-s_2}\right] & : ps_2 \geqslant 0, \\ \left(p\frac{1+s_2}{1-s_2}, p\frac{1-s_2}{1+s_2}\right) & : ps_2 < 0 \end{cases}$$

because $\mathrm{T}_2$ is positive (negative) semidefinite if and only if $p \geqslant 0$ ($p \leqslant 0$) holds. Therefore, the maximal eigenvalue $\lambda_M(\mathrm{T})$ of T is bounded from above by

$$\lambda_M(\mathrm{T}) \leqslant \begin{cases} s_1^2 + \frac{s_3^2}{1-s_2^2} - p + p\frac{1+s_2}{1-s_2} =: B_+ & : ps_2 \geqslant 0, \\ s_1^2 + \frac{s_3^2}{1-s_2^2} - p + p\frac{1-s_2}{1+s_2} =: B_- & : ps_2 < 0, \end{cases} \tag{60}$$

where the quantities $B_\pm$ are equivalent to

$$\begin{aligned} B_\pm &= s_1^2 + \frac{s_3^2}{1-s_2^2} - p + p\frac{1 \pm s_2}{1 \mp s_2} = s_1^2 + \frac{s_3^2}{1-s_2^2} \pm p\frac{2s_2}{1 \mp s_2} \\ &= s_1^2 + \frac{s_3^2}{1-s_2^2} \pm \frac{2s_1s_3}{1 \mp s_2} \pm \frac{2s_2s_3^2}{(1 \mp s_2)(1-s_2^2)} = s_1^2 + \frac{s_3^2 \mp s_2s_3^2 \pm 2s_2s_3^2}{(1 \mp s_2)(1-s_2^2)} \pm \frac{2s_1s_3}{1 \mp s_2} \\ &= s_1^2 + \frac{(1 \pm s_2)s_3^2}{(1 \mp s_2)(1-s_2)(1+s_2)} \pm \frac{2s_1s_3}{1 \mp s_2} = s_1^2 + \frac{s_3^2}{(1 \mp s_2)^2} \pm \frac{2s_1s_3}{1 \mp s_2} \\ &= \frac{s_1^2(1 \mp s_2)^2 + s_3^2 \pm 2(1 \mp s_2)s_1s_3}{(1 \mp s_2)^2} = \frac{\big(s_1(1 \mp s_2) \pm s_3\big)^2}{(1 \mp s_2)^2} \\ &= \frac{\big(f_1^{-1}e_1(1 \pm f_1^{-1}f_2) \pm f_1^{-1}(e_2 - f_1^{-1}f_2e_1)\big)^2}{(1 \pm f_1^{-1}f_2)^2} \\ &= \frac{(f_1^{-1}e_1 \pm f_1^{-2}f_2e_1 \pm f_1^{-1}e_2 \mp f_1^{-2}f_2e_1)^2}{(1 \pm f_1^{-1}f_2)^2} = \frac{(e_1 \pm e_2)^2}{(f_1 \pm f_2)^2}. \end{aligned}$$

Then the statement of the theorem follows because $ps_2 = \frac{\eta}{f_1^2(f_1^2 - f_2^2)}$ and $|f_1| > |f_2|$ while

$$\begin{aligned} 4\eta &= 4f_1^2e_1e_2 - 4f_1f_2e_2^2 - 4f_1f_2e_1^2 + 4e_1e_2f_2^2 \\ &= 4e_1e_2(f_1^2 + f_2^2) - 4f_1f_2(e_1^2 + e_2^2) \\ &= \big(2e_1e_2(f_1^2 + f_2^2) - 2f_1f_2(e_1^2 + e_2^2)\big) - \big(-2e_1e_2(f_1^2 + f_2^2) + 2f_1f_2(e_1^2 + e_2^2)\big) \\ &= \big(2e_1e_2(f_1^2 - 2f_1f_2 + f_2^2) - 2f_1f_2(e_1^2 + e_2^2) + (f_1^2 + f_2^2)(e_1^2 + e_2^2)\big) \\ &\quad - \big(-2e_1e_2(f_1^2 + 2f_1f_2 + f_2^2) + 2f_1f_2(e_1^2 + e_2^2) + (f_1^2 + f_2^2)(e_1^2 + e_2^2)\big) \\ &= (e_1^2 + 2e_1e_2 + e_2^2)(f_1^2 - 2f_1f_2 + f_2^2) - (e_1^2 - 2e_1e_2 + e_2^2)(f_1^2 + 2f_1f_2 + f_2^2) \\ &= (e_1 + e_2)^2(f_1 - f_2)^2 - (e_1 - e_2)^2(f_1 + f_2)^2. \end{aligned}$$

□

*Proof of Theorem 8.* First of all, we note that

$$\begin{aligned} \frac{2m_{ii} - (1-2\theta)\tau d_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}} - \frac{2}{3} &= \frac{6m_{ii} - 3(1-2\theta)\tau d_{ii} - (4+2\zeta)m_{ii} + 4(1-2\theta)\tau d_{ii}}{3\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)} \\ &= \frac{2(1-\zeta)m_{ii} + (1-2\theta)\tau d_{ii}}{3\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)}. \end{aligned}$$

Therefore, the value of $\omega_0$ is equal to $\frac{2}{3}$ if and only if

$$2(1-\zeta)m_{ii} + (1-2\theta)\tau d_{ii} \leqslant 0 \tag{61}$$

and, particularly, $\theta \geqslant \frac{1}{2}$ is mandatory. If condition (61) is satisfied and $d^{(\ell)} > d_{ii}$, the first argument of the maximum in (27b) is bounded from above by $\frac{1}{3}$ because

$$\begin{aligned}
\Big(\omega_0 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} - 1\Big) - \frac{1}{3} &= \Big(\frac{2}{3}\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} - 1\Big) - \frac{1}{3} \\
&= \frac{2\big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big) - 4\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)}{3\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \\
&= \frac{4\overbrace{(m^{(\ell)} - 2m_{ii})}^{\leqslant 0 \text{ by } (8)} + 2\overbrace{(1-2\theta)}^{\leqslant 0}\tau\overbrace{(2d_{ii} - d^{(\ell)})}^{\geqslant 0 \text{ by } (7)}}{3\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \leqslant 0, \\
\Big(1 - \omega_0 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}}\Big) - \frac{1}{3} &= \Big(1 - \frac{2}{3}\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}}\Big) - \frac{1}{3} \\
&= \frac{2\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big) - 2\big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big)}{3\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \\
&= \frac{4(m_{ii} - m^{(\ell)}) - 2(1-2\theta)\tau(d_{ii} - d^{(\ell)})}{3\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)},
\end{aligned}$$

which is nonpositive for finite differences due to the fact that $m_{ii} = m^{(\ell)} = 1$, $\theta \geqslant \frac{1}{2}$, and $d^{(\ell)} > d_{ii}$ while we have

$$\begin{aligned}
4(m_{ii} - m^{(\ell)}) - 2(1-2\theta)\tau(d_{ii} - d^{(\ell)}) &= 2(2s_\ell^2 - 1)m_{ii} - 2(1-2\theta)\tau(d_{ii} - d^{(\ell)}) \\
&= 2d_{ii}^{-1}\underbrace{(d^{(\ell)} - d_{ii})}_{\geqslant 0}\underbrace{\big(m_{ii} + (1-2\theta)\tau d_{ii}\big)}_{\leqslant 0 \text{ by } (61)} \leqslant 0
\end{aligned}$$

in the context of linear finite elements. On the other hand, the second argument is not greater than $\frac{1}{3}$ due to the fact that

$$\begin{aligned}
|1 - \tfrac{2}{3}d_{ii}^{-1}d^{(\ell)}| &= 1 - \tfrac{2}{3}d_{ii}^{-1}d^{(\ell)} \leqslant 1 - \tfrac{2}{3} = \tfrac{1}{3}, \quad \text{if } d^{(\ell)} \leqslant \tfrac{3}{2}d_{ii}, \\
|1 - \tfrac{2}{3}d_{ii}^{-1}d^{(\ell)}| &= \tfrac{2}{3}d_{ii}^{-1}d^{(\ell)} - 1 \leqslant \tfrac{4}{3} - 1 = \tfrac{1}{3}, \quad \text{if } d^{(\ell)} \geqslant \tfrac{3}{2}d_{ii}
\end{aligned}$$

by virtue of (7). Let us now assume that

$$2(1-\zeta)m_{ii} + (1-2\theta)\tau d_{ii} > 0. \tag{62}$$

Then the relaxation parameter $\omega_0$ attains the second argument of the maximum in (31) and, hence, the first expression in the definition of $B^{(\ell)}$ is bounded from above by $\frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}}$. Indeed, we have

$$\begin{aligned}
1 - \omega_0 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} &= \frac{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii} - \big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big)}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}} \\
&= \frac{(2-\zeta)m_{ii} + \overbrace{2\zeta m_{ii} - 2m^{(\ell)} + 4(1-s_\ell^2)(1-\zeta)m_{ii}}^{\overset{!}{=}0}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}} - \frac{2\overbrace{(1-s_\ell^2)}^{\geqslant 0}\overbrace{\big(2(1-\zeta)m_{ii} + (1-2\theta)\tau d_{ii}\big)}^{>0 \text{ by } (62)}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}} \\
&\leqslant \frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}}
\end{aligned}$$

because

$$2\zeta m_{ii} - 2m^{(\ell)} + 4(1-s_\ell^2)(1-\zeta)m_{ii} = \begin{cases} 2 - 2 = 0 & : \zeta = 1, \\ m_{ii}\big(1 - 3 + 2s_\ell^2 + 2(1-s_\ell^2)\big) = 0 & : \zeta = \frac{1}{2} \end{cases}$$

and, on the other hand,

$$\omega_0 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} - 1 = \frac{-(2+\zeta)m_{ii} + 2(1-2\theta)\tau d_{ii} + \big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big)}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}}$$
$$= \frac{(2-\zeta)m_{ii} - 4m_{ii} + 2(1-2\theta)\tau d_{ii} + \big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big)}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}}$$
$$\leqslant \frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}}$$

due to the fact that

$$4m_{ii} - 2(1-2\theta)\tau d_{ii} - \big(2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}\big)$$
$$= \begin{cases} 2\underbrace{\left(\zeta m_{ii} - (1-2\theta)\tau d_{ii}\right)}_{\geqslant 0 \text{ by (10)}} + 2\underbrace{\left((2-\zeta)m_{ii} - m^{(\ell)}\right)}_{\geqslant 0 \text{ by (8)}} + \underbrace{(1-2\theta)\tau d^{(\ell)}}_{\geqslant 0} \geqslant 0 & : \theta \leqslant \frac{1}{2}, \\ 2\underbrace{\left(2m_{ii} - m^{(\ell)}\right)}_{\geqslant 0 \text{ by (8)}} - \underbrace{(1-2\theta)}_{\leqslant 0}\tau\underbrace{\left(2d_{ii} - d^{(\ell)}\right)}_{\geqslant 0 \text{ by (7)}} \geqslant 0 & : \theta > \frac{1}{2}. \end{cases}$$

Finally, the second argument of the maximum in (27b) satisfies

$$1 - \omega_0 \frac{d^{(\ell)}}{d_{ii}} = 1 - \frac{2m_{ii}d^{(\ell)} - (1-2\theta)\tau d_{ii}d^{(\ell)}}{d_{ii}\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)}$$
$$= \frac{(2+\zeta)m_{ii}d_{ii} - 2(1-2\theta)\tau d_{ii}^2 - 2m_{ii}d^{(\ell)} + (1-2\theta)\tau d_{ii}d^{(\ell)}}{d_{ii}\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)}$$
$$= \frac{(2-\zeta)m_{ii}d_{ii} + \overbrace{\big(2(1-\zeta)m_{ii} + (1-2\theta)\tau d_{ii}\big)}^{\geqslant 0 \text{ by (62)}}\overbrace{\big(d^{(\ell)} - 2d_{ii}\big)}^{\leqslant 0} + \overbrace{(4-2\zeta)}^{\geqslant 0} m_{ii}\overbrace{\big(d_{ii} - d^{(\ell)}\big)}^{\leqslant 0}}{d_{ii}\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)}$$
$$\leqslant \frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}},$$

$$\omega_0 \frac{d^{(\ell)}}{d_{ii}} - 1 = \frac{2m_{ii}d^{(\ell)} - (1-2\theta)\tau d_{ii}d^{(\ell)} - (2+\zeta)m_{ii}d_{ii} + 2(1-2\theta)\tau d_{ii}^2}{d_{ii}\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)}$$
$$= \frac{(2-\zeta)m_{ii}d_{ii} + \overbrace{\big(d^{(\ell)} - 2d_{ii}\big)}^{\leqslant 0 \text{ by (7)}}\overbrace{\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)}^{\geqslant 0 \text{ by (10)}}}{d_{ii}\big((2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}\big)} \leqslant \frac{(2-\zeta)m_{ii}}{(2+\zeta)m_{ii} - 2(1-2\theta)\tau d_{ii}},$$

which proves the validity of inequality (32).

To prove identity (33), we have to show the validity of

$$\left|1 - \omega \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}}\right| \leqslant 1 - \omega d_{ii}^{-1} d^{(\ell)}$$

whenever $d^{(\ell)} \leqslant d_{ii}$ and $\omega \in (0, 1]$. For this purpose, we first note that

$$(1 - \omega d_{ii}^{-1} d^{(\ell)}) - \Big(1 - \omega \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}}\Big) = \omega \Big(\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} - d_{ii}^{-1} d^{(\ell)}\Big)$$
$$= \omega \frac{2d_{ii}m^{(\ell)} - (1-2\theta)\tau d_{ii}d^{(\ell)} - 2m_{ii}d^{(\ell)} + (1-2\theta)\tau d_{ii}d^{(\ell)}}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} = \omega \frac{2(d_{ii}m^{(\ell)} - m_{ii}d^{(\ell)})}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \geqslant 0$$

due to the fact that

$$m^{(\ell)}d_{ii} - m_{ii}d^{(\ell)} = d_{ii} - d^{(\ell)} \geqslant 0 \qquad \text{if } \zeta = 1,$$
$$m^{(\ell)}d_{ii} - m_{ii}d^{(\ell)} = m_{ii}(\tfrac{3}{2} - s_\ell^2)d_{ii} - m_{ii}2d_{ii}s_\ell^2 = \tfrac{3}{2}m_{ii}d_{ii}(1 - 2s_\ell^2) = \tfrac{3}{2}m_{ii}(d_{ii} - d^{(\ell)}) \geqslant 0 \quad \text{if } \zeta = \tfrac{1}{2}.$$

On the other hand, we have

$$
\begin{aligned}
&(1-\omega d_{ii}^{-1} d^{(\ell)}) - \Big(\omega \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2m_{ii} - (1-2\theta)\tau d_{ii}} - 1\Big) \\
&\quad = 2 - \omega \frac{2m_{ii} d^{(\ell)} - (1-2\theta)\tau d_{ii} d^{(\ell)} + 2 d_{ii} m^{(\ell)} - (1-2\theta)\tau d_{ii} d^{(\ell)}}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \\
&\quad = 2 \frac{2m_{ii} d_{ii} - (1-2\theta)\tau d_{ii}^2 - \omega(m_{ii} d^{(\ell)} + d_{ii} m^{(\ell)}) + \omega(1-2\theta)\tau d_{ii} d^{(\ell)}}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} \\
&\quad = 2 \frac{(2-\zeta) m_{ii} d_{ii} - \omega\big((1-\zeta) m_{ii} d^{(\ell)} + d_{ii} m^{(\ell)}\big)}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)} + \frac{\overbrace{\big(\zeta m_{ii} - (1-2\theta)\tau d_{ii}\big)}^{\geqslant 0 \text{ by } (10)} \overbrace{(d_{ii} - \omega d^{(\ell)})}^{\geqslant d_{ii} - d^{(\ell)} \geqslant 0}}{d_{ii}\big(2m_{ii} - (1-2\theta)\tau d_{ii}\big)},
\end{aligned}
$$

which is nonnegative either for $\zeta = m_{ii} = m^{(\ell)} = 1$ in case of finite differences or according to

$$
(2-\zeta) m_{ii} d_{ii} - \omega\big((1-\zeta) m_{ii} d^{(\ell)} + d_{ii} m^{(\ell)}\big) = m_{ii} d_{ii}\Big(\tfrac{3}{2} - \omega(s_\ell^2 + \tfrac{3}{2} - s_\ell^2)\Big) = \tfrac{3}{2} m_{ii} d_{ii}(1-\omega) \geqslant 0
$$

for linear finite elements and $\zeta = \frac{1}{2}$. □

Although the statement of Theorem 11 is true for finite element and finite difference discretizations, we prove the result by considering both spatial discretization techniques individually.

*Proof of Theorem 11 for finite differences.* To prove that $\operatorname{spr}\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu\big)$ is smaller than 1 for all $\ell = 1, \ldots, \bar{N}$, we directly estimate the eigenvalues $\lambda_\pm \in \mathbb{C}$ of $\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu$ which are the roots of the characteristic polynomial $p : \mathbb{C} \to \mathbb{C}$

$$
\begin{aligned}
p(\lambda) &= \det\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu - \lambda \mathrm{I}\big) \\
&= (\bar{a}^{(\ell)})^{-2} \det \begin{pmatrix} (\bar{a}^{(\ell)} - c_\ell^4 a^{(\ell)})(j^{(\mathrm{Jac},\ell)})^\nu - \bar{a}^{(\ell)}\lambda & s_\ell^2 c_\ell^2 a^{(N+1-\ell)}(j^{(\mathrm{Jac},N+1-\ell)})^\nu \\ s_\ell^2 c_\ell^2 a^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu & (\bar{a}^{(\ell)} - s_\ell^4 a^{(N+1-\ell)})(j^{(\mathrm{Jac},N+1-\ell)})^\nu - \bar{a}^{(\ell)}\lambda \end{pmatrix} \\
&= (\bar{a}^{(\ell)})^{-2}\Big(\big((\bar{a}^{(\ell)} - c_\ell^4 a^{(\ell)})(j^{(\mathrm{Jac},\ell)})^\nu - \bar{a}^{(\ell)}\lambda\big)\big((\bar{a}^{(\ell)} - s_\ell^4 a^{(N+1-\ell)})(j^{(\mathrm{Jac},N+1-\ell)})^\nu - \bar{a}^{(\ell)}\lambda\big) \\
&\qquad - s_\ell^4 c_\ell^4 a^{(\ell)} a^{(N+1-\ell)}(j^{(\mathrm{Jac},\ell)})^\nu (j^{(\mathrm{Jac},N+1-\ell)})^\nu\Big) \\
&= (\bar{a}^{(\ell)})^{-2}\Big((\bar{a}^{(\ell)}\lambda)^2 - \bar{a}^{(\ell)}\lambda\big((\bar{a}^{(\ell)} - c_\ell^4 a^{(\ell)})(j^{(\mathrm{Jac},\ell)})^\nu + (\bar{a}^{(\ell)} - s_\ell^4 a^{(N+1-\ell)})(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) \\
&\qquad + \big((\bar{a}^{(\ell)})^2 - \bar{a}^{(\ell)}(c_\ell^4 a^{(\ell)} + s_\ell^4 a^{(N+1-\ell)})\big)(j^{(\mathrm{Jac},\ell)})^\nu (j^{(\mathrm{Jac},N+1-\ell)})^\nu\Big) \\
&= (\bar{a}^{(\ell)})^{-2}\Big((\bar{a}^{(\ell)}\lambda)^2 - \bar{a}^{(\ell)}\lambda\big(s_\ell^2(\bar{a}^{(\ell)} + c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar{a}^{(\ell)} + s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) \\
&\qquad + 2 s_\ell^2 c_\ell^2 \bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu (j^{(\mathrm{Jac},N+1-\ell)})^\nu\Big).
\end{aligned}
$$

Here, the last identity is valid because

$$
\bar{a}^{(\ell)} - c_\ell^4 a^{(\ell)} = 1 + 2\theta\tau d_{ii} s_\ell^2 c_\ell^2 - c_\ell^4 - 2\theta\tau d_{ii} s_\ell^2 c_\ell^4 = s_\ell^2 + c_\ell^2 - c_\ell^4 + 2\theta\tau s_\ell^4 c_\ell^2 = s_\ell^2(\bar{a}^{(\ell)} + c_\ell^2), \tag{63a}
$$

$$
\bar{a}^{(\ell)} - s_\ell^4 a^{(N+1-\ell)} = 1 + 2\theta\tau d_{ii} s_\ell^2 c_\ell^2 - s_\ell^4 - 2\theta\tau d_{ii} s_\ell^4 c_\ell^2 = s_\ell^2 + c_\ell^2 - s_\ell^4 + 2\theta\tau s_\ell^2 c_\ell^4 = c_\ell^2(\bar{a}^{(\ell)} + s_\ell^2). \tag{63b}
$$

Therefore, the eigenvalues $\lambda_\pm$ satisfy

$$
\begin{aligned}
&\Big(\bar{a}^{(\ell)}\lambda_\pm - \tfrac{1}{2}\big(s_\ell^2(\bar{a}^{(\ell)} + c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar{a}^{(\ell)} + s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)\Big)^2 \\
&\quad = \tfrac{1}{4}\big(s_\ell^2(\bar{a}^{(\ell)} + c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar{a}^{(\ell)} + s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 - 2 s_\ell^2 c_\ell^2 \bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu (j^{(\mathrm{Jac},N+1-\ell)})^\nu.
\end{aligned} \tag{64}
$$

Let us now consider the special case $(j^{(\mathrm{Jac},\ell)})^\nu (j^{(\mathrm{Jac},N+1-\ell)})^\nu \leqslant 0$. Then the right hand side of (64) is obviously nonnegative and can be estimated by

$$\begin{aligned} 0 &\leqslant \tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 - 2s_\ell^2c_\ell^2\bar a^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu \\ &= \tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu\big)^2 + \tfrac14\big(c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 \\ &\quad + s_\ell^2c_\ell^2\underbrace{(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu}_{\leqslant 0}\underbrace{\big(\tfrac12(\bar a^{(\ell)}+c_\ell^2)(\bar a^{(\ell)}+s_\ell^2)-2\bar a^{(\ell)}\big)}_{>-\frac12(\bar a^{(\ell)}+c_\ell^2)(\bar a^{(\ell)}+s_\ell^2)} \\ &\leqslant \tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu - c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 \end{aligned} \tag{65}$$

because

$$(\bar a^{(\ell)}+c_\ell^2)(\bar a^{(\ell)}+s_\ell^2)-2\bar a^{(\ell)} = (\bar a^{(\ell)})^2-\bar a^{(\ell)}+s_\ell^2c_\ell^2 = \bar a^{(\ell)}\underbrace{(\bar a^{(\ell)}-1)}_{=\theta\tau\bar d^{(\ell)}}+s_\ell^2c_\ell^2>0. \tag{66}$$

Thus, both eigenvalues are real and satisfy

$$\begin{aligned} \bar a^{(\ell)}|\lambda_\pm| &\leqslant \tfrac12\big|s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big| \\ &\quad + \tfrac12\big|s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu - c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big| \\ &= \tfrac12\big|s_\ell^2(\bar a^{(\ell)}+c_\ell^2)|j^{(\mathrm{Jac},\ell)}|^\nu - c_\ell^2(\bar a^{(\ell)}+s_\ell^2)|j^{(\mathrm{Jac},N+1-\ell)}|^\nu\big| \\ &\quad + \tfrac12\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)|j^{(\mathrm{Jac},\ell)}|^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)|j^{(\mathrm{Jac},N+1-\ell)}|^\nu\big) \\ &= \max\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)|j^{(\mathrm{Jac},\ell)}|^\nu, c_\ell^2(\bar a^{(\ell)}+s_\ell^2)|j^{(\mathrm{Jac},N+1-\ell)}|^\nu\big) \\ &\leqslant \bar a^{(\ell)}\max\big(|j^{(\mathrm{Jac},\ell)}|^\nu, |j^{(\mathrm{Jac},N+1-\ell)}|^\nu\big) < \bar a^{(\ell)} \end{aligned}$$

due to the reverse triangle inequality, Theorem 5, (63) and the fact that $(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu \leqslant 0$.

On the other hand, for $(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu > 0$, we can assume that

$$j_{\max} \coloneqq \max\big((j^{(\mathrm{Jac},\ell)})^\nu, (j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) > 0.$$

Otherwise, consider $-(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu$ instead of $(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu$. Then estimate (66) can be exploited as in (65) to prove

$$\begin{aligned} &\tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 - 2s_\ell^2c_\ell^2\bar a^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu \\ &\quad > \tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu - c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 \geqslant 0 \end{aligned} \tag{67}$$

and, hence, both eigenvalues are real and positive because

$$\begin{aligned} \bar a^{(\ell)}\lambda_\pm &> \tfrac12\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) \\ &\quad - \tfrac12\big|s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu - c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big| \\ &= \min\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu, c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) \geqslant 0 \end{aligned}$$

by (64) and (67). Furthermore, the maximal eigenvalue $\lambda_+$ satisfies

$$\begin{aligned} \bar a^{(\ell)}\lambda_+ &= \tfrac12\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big) \\ &\quad + \sqrt{\tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2 - 2s_\ell^2c_\ell^2\bar a^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu} \\ &\leqslant \tfrac12\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)j_{\max} + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)j_{\max}\big) \\ &\quad + \sqrt{\tfrac14\big(s_\ell^2(\bar a^{(\ell)}+c_\ell^2)j_{\max} + c_\ell^2(\bar a^{(\ell)}+s_\ell^2)j_{\max}\big)^2 - 2s_\ell^2c_\ell^2\bar a^{(\ell)}j_{\max}^2} \\ &= \tfrac12(\bar a^{(\ell)}+2s_\ell^2c_\ell^2)j_{\max} + \sqrt{\tfrac14(\bar a^{(\ell)}+2s_\ell^2c_\ell^2)^2 - 2s_\ell^2c_\ell^2\bar a^{(\ell)}}\,j_{\max} \\ &= \tfrac12(\bar a^{(\ell)}+2s_\ell^2c_\ell^2)j_{\max} + \tfrac12|\bar a^{(\ell)}-2s_\ell^2c_\ell^2|j_{\max} = \max(\bar a^{(\ell)}, 2s_\ell^2c_\ell^2)j_{\max} < \bar a^{(\ell)} \end{aligned} \tag{68}$$

by Theorem 5 and due to the fact that $2s_\ell^2c_\ell^2 \leqslant \frac{1}{2} \leqslant 1 \leqslant \bar{a}^{(\ell)}$ because $\lambda_+$ grows monotonically with respect to $(j^{(\mathrm{Jac},\ell)})^\nu$ and $(j^{(\mathrm{Jac},N+1-\ell)})^\nu$. Indeed, for instance, we have

$$
\begin{aligned}
\bar{a}^{(\ell)}\frac{\partial\lambda_+}{\partial(j^{(\mathrm{Jac},N+1-\ell)})^\nu} &= \tfrac{1}{2}c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)\\
&\quad+\frac{\frac{1}{2}\Big(\frac{1}{2}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu\Big)}{\sqrt{\frac{1}{4}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu}}\\
&\geqslant\frac{\frac{1}{4}c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)\big|s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu-c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big|}{\sqrt{\frac{1}{4}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu}}\\
&\quad+\frac{\frac{1}{2}\Big(\frac{1}{2}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu\Big)}{\sqrt{\frac{1}{4}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)^2-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu(j^{(\mathrm{Jac},N+1-\ell)})^\nu}}
\end{aligned}
$$

by (67), which is nonnegative because

$$
\begin{aligned}
&\tfrac{1}{2}c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)\big|s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu-c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big|\\
&\quad+\tfrac{1}{2}\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu\\
&\quad=c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)\max\big(s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu,c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\big)-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu\\
&\quad\geqslant c_\ell^2(\bar{a}^{(\ell)}+s_\ell^2)s_\ell^2(\bar{a}^{(\ell)}+c_\ell^2)(j^{(\mathrm{Jac},\ell)})^\nu-2s_\ell^2c_\ell^2\bar{a}^{(\ell)}(j^{(\mathrm{Jac},\ell)})^\nu\\
&\quad=s_\ell^2c_\ell^2(j^{(\mathrm{Jac},\ell)})^\nu\big((\bar{a}^{(\ell)}+s_\ell^2)(\bar{a}^{(\ell)}+c_\ell^2)-2\bar{a}^{(\ell)}\big)\geqslant 0
\end{aligned}
$$

according to (66). This proves the statement of Theorem 11 for finite differences by exploiting (45). □

*Proof of Theorem 11 for finite elements.* For finite elements, we first note that $\mathrm{J}^{(\mathrm{Cor},\ell)}$ is singular because

$$
\begin{aligned}
(\bar{a}^{(\ell)})^2\det(\mathrm{J}^{(\mathrm{Cor},\ell)}) &= (\bar{a}^{(\ell)})^2\det\left(\begin{pmatrix}1-\zeta^{-1}c_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(\ell)} & \zeta^{-1}s_\ell^2c_\ell^2(\bar{a}^{(\ell)})^{-1}a^{(N+1-\ell)}\\ \zeta^{-1}s_\ell^2c_\ell^2(\bar{a}^{(\ell)})^{-1}a^{(\ell)} & 1-\zeta^{-1}s_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(N+1-\ell)}\end{pmatrix}\right)\\
&= (\bar{a}^{(\ell)}-2c_\ell^4a^{(\ell)})(\bar{a}^{(\ell)}-2s_\ell^4a^{(N+1-\ell)})-4s_\ell^4c_\ell^4a^{(\ell)}a^{(N+1-\ell)}\\
&= \bar{a}^{(\ell)}(\bar{a}^{(\ell)}-2s_\ell^4a^{(N+1-\ell)}-2c_\ell^4a^{(\ell)}) = 0
\end{aligned}
$$

according to

$$
\begin{aligned}
2s_\ell^4a^{(N+1-\ell)}+2c_\ell^4a^{(\ell)} &= m_{ii}(3s_\ell^4-2s_\ell^4c_\ell^2+3c_\ell^4-2s_\ell^2c_\ell^4)+\theta\tau d_{ii}(4s_\ell^4c_\ell^2+4s_\ell^2c_\ell^4)\\
&= m_{ii}(3-8s_\ell^2c_\ell^2)+\theta\tau d_{ii}(4s_\ell^2c_\ell^2) = \bar{m}^{(\ell)}+\theta\tau\bar{d}^{(\ell)} = \bar{a}^{(\ell)}.
\end{aligned}
\tag{69}
$$

Therefore, the matrix $\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^{\nu_1+\nu_2}$ has a vanishing eigenvalue, too, and its spectral radius coincides with the absolute value of the trace, that is,

$$
\begin{aligned}
\mathrm{spr}\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu\big) &= \Big|\mathrm{tr}\big(\mathrm{J}^{(\mathrm{Cor},\ell)}(\mathrm{J}^{(\mathrm{Jac},\ell)})^\nu\big)\Big|\\
&= \Big|\big(1-2c_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(\ell)}\big)(j^{(\mathrm{Jac},\ell)})^\nu+\big(1-2s_\ell^4(\bar{a}^{(\ell)})^{-1}a^{(N+1-\ell)}\big)(j^{(\mathrm{Jac},N+1-\ell)})^\nu\Big|\\
&= 2(\bar{a}^{(\ell)})^{-1}\Big|s_\ell^4a^{(N+1-\ell)}(j^{(\mathrm{Jac},\ell)})^\nu+c_\ell^4a^{(\ell)}(j^{(\mathrm{Jac},N+1-\ell)})^\nu\Big|\\
&\leqslant 2(\bar{a}^{(\ell)})^{-1}\Big(s_\ell^4a^{(N+1-\ell)}|j^{(\mathrm{Jac},\ell)}|^\nu+c_\ell^4a^{(\ell)}|j^{(\mathrm{Jac},N+1-\ell)}|^\nu\Big)\\
&< 2(\bar{a}^{(\ell)})^{-1}\Big(s_\ell^4a^{(N+1-\ell)}+c_\ell^4a^{(\ell)}\Big) = 1
\end{aligned}
\tag{70}
$$

by virtue of (25) and (69). This proves the statement of Theorem 11 for finite elements by exploiting (45). □

*Proof of Lemma 12.* To prove the inequalities, we first note that

$$2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)} \geqslant \tfrac{3}{2}m_{ii} > 0, \quad \ell = 1,\dots,\bar{N} \tag{71}$$

because

$$\begin{aligned} 2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)} &= m_{ii}(6 - 16s_\ell^2c_\ell^2 - 2s_\ell^2c_\ell^2) + 2s_\ell^2c_\ell^2\underbrace{\left(m_{ii} - 2(1-2\theta)\tau d_{ii}\right)}_{\geqslant 0 \text{ by } (10)} \\ &\geqslant 6m_{ii}(1-3s_\ell^2c_\ell^2) \geqslant 6m_{ii}(1-\tfrac{3}{4}) \geqslant \tfrac{3}{2}m_{ii} \quad \text{if } \zeta = \tfrac{1}{2}, \end{aligned} \tag{72}$$

$$\begin{aligned} 2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)} &= 2(1 - s_\ell^2c_\ell^2) + 2s_\ell^2c_\ell^2\underbrace{\left(1 - (1-2\theta)\tau d_{ii}\right)}_{\geqslant 0 \text{ by } (10)} \\ &\geqslant 2(1-s_\ell^2c_\ell^2) \geqslant 2(1-\tfrac{1}{4}) \geqslant \tfrac{3}{2} \quad \text{if } \zeta = 1, \end{aligned} \tag{73}$$

due to the fact that $s_\ell^2c_\ell^2 \in (0, \frac{1}{4}]$. We now find upper bounds for the spectral norm of the submatrices by using Theorem 3, where different values for $e_1$ and $e_2$ are considered while

$$f_1 = \bar{m}^{(\ell)} + \theta\tau\bar{d}^{(\ell)}, \quad f_2 = -\bar{m}^{(\ell)} + (1-\theta)\tau\bar{d}^{(\ell)}.$$

Indeed, the requirement $|f_2| < |f_1|$ made in this theorem is valid because

$$f_2^2 - f_1^2 = -\tau\bar{d}^{(\ell)}\underbrace{\left(2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}\right)}_{>0 \text{ by } (71)} < 0,$$

which can be shown as in (30).

- Then, according to Theorem 3, the spectral norm of $\mathrm{I}_K - \zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}$ is bounded from above by

  $$\|\mathrm{I}_K - \zeta^{-1}c_\ell^4(\bar{\mathrm{S}}_K^{(\ell)})^{-1}\mathrm{S}_K^{(\ell)}\|_2 \leqslant \max\left(\left|1 - \zeta^{-1}c_\ell^4\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}}\right|, \left|\frac{\bar{d}^{(\ell)} - \zeta^{-1}c_\ell^4 d^{(\ell)}}{\bar{d}^{(\ell)}}\right|\right)$$

  using the quantities

  $$\begin{aligned} e_1 &= (\bar{m}^{(\ell)} + \theta\tau\bar{d}^{(\ell)}) - \zeta^{-1}c_\ell^4(m^{(\ell)} + \theta\tau d^{(\ell)}), \\ e_2 &= \left(-\bar{m}^{(\ell)} + (1-\theta)\tau\bar{d}^{(\ell)}\right) - \zeta^{-1}c_\ell^4\left(-m^{(\ell)} + (1-\theta)\tau d^{(\ell)}\right). \end{aligned}$$

  This bound can be simplified by exploiting the identities

  $$\frac{\bar{d}^{(\ell)} - \zeta^{-1}c_\ell^4 d^{(\ell)}}{\bar{d}^{(\ell)}} = \frac{\bar{d}^{(\ell)} - c_\ell^2\bar{d}^{(\ell)}}{\bar{d}^{(\ell)}} = 1 - c_\ell^2 = s_\ell^2$$

  due to (39) and

  $$\begin{aligned} 1 - \zeta^{-1}c_\ell^4\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}} &= 1 - c_\ell^4 + \zeta^{-1}c_\ell^4\frac{2(\zeta\bar{m}^{(\ell)} - m^{(\ell)}) - (1-2\theta)\tau(\zeta\bar{d}^{(\ell)} - d^{(\ell)})}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}} \\ &= 1 - c_\ell^4 + \zeta^{-1}c_\ell^4\frac{2(\zeta\bar{m}^{(\ell)} - m^{(\ell)}) + 2(1-2\theta)\tau s_\ell^4 d_{ii}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}}, \end{aligned} \tag{74}$$

  where the numerator of the last fraction is nonpositive if $\theta \geqslant \frac{1}{2}$ by (38) or due to the fact that

  $$\begin{aligned} 2\zeta\bar{m}^{(\ell)} - 2m^{(\ell)} + 2\zeta s_\ell^4 m_{ii} - 2s_\ell^4\overbrace{\left(\zeta m_{ii} - (1-2\theta)\tau d_{ii}\right)}^{\geqslant 0 \text{ by } (10)} &\leqslant m_{ii}(3 - 8s_\ell^2c_\ell^2 - 3 + 2s_\ell^2 + s_\ell^4) \\ &= 3m_{ii}s_\ell^2(3s_\ell^2 - 2) \leqslant 0 \end{aligned} \tag{75}$$

for finite elements because $s_\ell^2 \leqslant \frac{1}{2}$ for all $\ell = 1, \ldots, \bar{N}$. For $\zeta = 1$ (and $\theta < \frac{1}{2}$), we observe

$$1 - \zeta^{-1} c_\ell^4 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} = 1 - c_\ell^4 + c_\ell^4 \frac{2s_\ell^4 - 2s_\ell^4 \overbrace{\big(1 - (1-2\theta)\tau d_{ii}\big)}^{\geqslant 0 \text{ by } (10)}}{2 - 2s_\ell^2 c_\ell^2 + 2s_\ell^2 c_\ell^2 \big(1 - (1-2\theta)\tau d_{ii}\big)}$$
$$\leqslant 1 - c_\ell^4 + c_\ell^4 \frac{2s_\ell^4}{2(1 - s_\ell^2 c_\ell^2)} = 1 - c_\ell^4 \frac{1 - s_\ell^2(c_\ell^2 + s_\ell^2)}{1 - s_\ell^2 c_\ell^2} = 1 - \frac{c_\ell^6}{1 - s_\ell^2 c_\ell^2} \leqslant 1 - c_\ell^6.$$

On the other hand, we have

$$1 - \zeta^{-1} c_\ell^4 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}}$$
$$= 1 - c_\ell^2 \frac{2c_\ell^2 - (1-2\theta)\tau c_\ell^2 d^{(\ell)}}{2 - (1-2\theta)\tau \bar{d}^{(\ell)}} \geqslant 1 - c_\ell^2 \frac{2 - (1-2\theta)\tau \bar{d}^{(\ell)}}{2 - (1-2\theta)\tau \bar{d}^{(\ell)}} = 1 - c_\ell^2 \geqslant 0 \quad \text{if } \zeta = 1,$$
$$1 - \zeta^{-1} c_\ell^4 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} = \frac{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)} - 4c_\ell^4 m^{(\ell)} + 2c_\ell^4(1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}}$$
$$= \frac{2(\bar{m}^{(\ell)} - 2c_\ell^4 m^{(\ell)}) - (1-2\theta)\tau d_{ii}(4s_\ell^2 c_\ell^2 - 4c_\ell^4 s_\ell^2)}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}}$$
$$= \frac{2(\bar{m}^{(\ell)} - 2c_\ell^4 m^{(\ell)} - s_\ell^4 c_\ell^2 m_{ii}) + 2s_\ell^4 c_\ell^2 \overbrace{(m_{ii} - 2(1-2\theta)\tau d_{ii})}^{\geqslant 0 \text{ by } (10)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}}$$
$$\geqslant \frac{2m_{ii}(3 - 8s_\ell^2 c_\ell^2 - 3c_\ell^4 + 2s_\ell^2 c_\ell^4 - s_\ell^4 c_\ell^2)}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} = \frac{6m_{ii} s_\ell^6}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \geqslant 0 \quad \text{if } \zeta = \tfrac{1}{2}$$

according to (71).

- To estimate the spectral norm of $\mathrm{I}_K - \zeta^{-1} s_\ell^4 (\bar{\mathrm{S}}_K^{(\ell)})^{-1} \mathrm{S}_K^{(N+1-\ell)}$, we can proceed similarly by replacing $m^{(\ell)}$ and $d^{(\ell)}$ by $m^{(N+1-\ell)}$ and $d^{(N+1-\ell)}$, respectively, while $s_\ell^2$ has to be substituted by $c_\ell^2$ and vice versa. However, the numerator occurring in (74) does not have to be nonpositive for $\zeta = \frac{1}{2}$ and $\theta \geqslant \frac{1}{2}$ while the last inequality of (75) is not valid any more either. However, using the same ideas, we derive

$$1 - \zeta^{-1} s_\ell^4 \frac{2m^{(N+1-\ell)} - (1-2\theta)\tau d^{(N+1-\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \leqslant 1 - s_\ell^4 + s_\ell^4 \frac{6m_{ii} c_\ell^2 (3c_\ell^2 - 2)}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \tag{76}$$
$$\leqslant 1 - s_\ell^4 + s_\ell^4 \frac{6m_{ii} c_\ell^2 (3c_\ell^2 - 2)}{6m_{ii}(1 - 3s_\ell^2 c_\ell^2)} = 1 - s_\ell^4 \frac{1 - 3c_\ell^2(s_\ell^2 + c_\ell^2) + 2c_\ell^2}{1 - 3s_\ell^2 c_\ell^2} \leqslant 1 - s_\ell^6 \tag{77}$$

for $\zeta = \frac{1}{2}$, $\theta \in [0, 1]$, and $c_\ell^2 \geqslant \frac{2}{3}$, because estimate (76) can be shown as in (74) and (75) while the first inequality in (77) is valid due to (72). For $\zeta = \frac{1}{2}$, $\theta \in [0, 1]$, and $c_\ell^2 < \frac{2}{3}$, the same inequality can be easily verified because

$$1 - \zeta^{-1} s_\ell^4 \frac{2m^{(N+1-\ell)} - (1-2\theta)\tau d^{(N+1-\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \leqslant 1 - s_\ell^4 + s_\ell^4 \frac{6m_{ii} c_\ell^2 (3c_\ell^2 - 2)}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \leqslant 1 - s_\ell^4 \leqslant 1 - s_\ell^6.$$

- Invoking Theorem 3 using $e_1 = m^{(\ell)} + \theta\tau d^{(\ell)}$ and $e_2 = -m^{(\ell)} + (1-\theta)\tau d^{(\ell)}$, an upper bound of $\big\|\zeta^{-1} s_\ell^2 c_\ell^2 (\bar{\mathrm{S}}_K^{(\ell)})^{-1} \mathrm{S}_K^{(\ell)}\big\|_2$ is given by

$$\|\zeta^{-1} s_\ell^2 c_\ell^2 (\bar{\mathrm{S}}_K^{(\ell)})^{-1} \mathrm{S}_K^{(\ell)}\|_2 \leqslant \zeta^{-1} s_\ell^2 c_\ell^2 \max\left(\left|\frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}}\right|, \left|\frac{d^{(\ell)}}{\bar{d}^{(\ell)}}\right|\right), \tag{78}$$

where

$$\zeta^{-1} s_\ell^2 c_\ell^2 \frac{d^{(\ell)}}{\bar{d}^{(\ell)}} = \zeta^{-1} s_\ell^2 c_\ell^2 \frac{2s_\ell^2 d_{ii}}{2\zeta^{-1} s_\ell^2 c_\ell^2 d_{ii}} = s_\ell^2.$$

Furthermore, it is not necessary to take the absolute value of the first argument in the definition of the maximum in (78) because

$$\zeta^{-1} s_\ell^2 c_\ell^2 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} \geqslant 0$$

by (13) and (71). On the other hand, the expression is bounded from above by $s_\ell^2$ for a finite difference approximation, that is, $\zeta = 1$, because

$$\begin{aligned}\zeta^{-1} s_\ell^2 c_\ell^2 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} - s_\ell^2 &= s_\ell^2 \frac{2c_\ell^2 - (1-2\theta)\tau c_\ell^2 d^{(\ell)} - 2 + (1-2\theta)\tau \bar{d}^{(\ell)}}{2 - (1-2\theta)\tau \bar{d}^{(\ell)}} \\ &= s_\ell^2 \frac{-2s_\ell^2}{2 - (1-2\theta)\tau \bar{d}^{(\ell)}} \leqslant 0\end{aligned}$$

while, in case of finite elements, an upper bound is given by $\frac{4}{3} s_\ell^2$ due to

$$\begin{aligned}&\zeta^{-1} s_\ell^2 c_\ell^2 \frac{2m^{(\ell)} - (1-2\theta)\tau d^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau \bar{d}^{(\ell)}} - \frac{s_\ell^2 c_\ell^4}{1 - 3s_\ell^2 c_\ell^2} \\ &= \frac{4(1-3s_\ell^2c_\ell^2)s_\ell^2c_\ell^2 m^{(\ell)} - 2s_\ell^2 c_\ell^4 \bar{m}^{(\ell)} - (1-2\theta)\tau\big(2(1-3s_\ell^2c_\ell^2)s_\ell^2c_\ell^2 d^{(\ell)} - s_\ell^2 c_\ell^4 \bar{d}^{(\ell)}\big)}{(1-3s_\ell^2c_\ell^2)(2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)})} \\ &= s_\ell^2 c_\ell^2 \frac{m_{ii}(6 - 4s_\ell^2 - 18 s_\ell^2 c_\ell^2 + 12 s_\ell^4 c_\ell^2 - 6c_\ell^2 + 16 s_\ell^2 c_\ell^4) - 2m_{ii}(s_\ell^2 - 3s_\ell^4 c_\ell^2 - s_\ell^2 c_\ell^4)}{(1-3s_\ell^2c_\ell^2)(2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)})} \\ &\quad + s_\ell^2 c_\ell^2 \overbrace{(s_\ell^2 - 3s_\ell^4 c_\ell^2 - s_\ell^2 c_\ell^4)}^{=s_\ell^2((1-3s_\ell^2c_\ell^2)-c_\ell^4)\leqslant 0 \text{ by } (79)} \frac{\overbrace{2m_{ii} - 4(1-2\theta)\tau d_{ii}}^{\geqslant 0 \text{ by } (10)}}{(1-3s_\ell^2c_\ell^2)(2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)})} \\ &\leqslant s_\ell^2 c_\ell^2 \frac{m_{ii}(6 - 18 s_\ell^2 c_\ell^2 - 6(s_\ell^2 + c_\ell^2) + 18 s_\ell^4 c_\ell^2 + 18 s_\ell^2 c_\ell^4)}{(1-3s_\ell^2c_\ell^2)(2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)})} = 0\end{aligned}$$

by virtue of the fact that

$$\begin{aligned}\frac{c_\ell^4}{1-3s_\ell^2c_\ell^2} = \frac{3(1-s_\ell^2)^2}{3(1-3s_\ell^2c_\ell^2)} = \frac{3 - 6s_\ell^2 + 3s_\ell^4}{3(1-3s_\ell^2c_\ell^2)} &= \frac{4 - 12 s_\ell^2 \overbrace{(1-s_\ell^2)}^{=c_\ell^2} - \overbrace{(1-3s_\ell^2)^2}^{\geqslant 0}}{3(1-3s_\ell^2c_\ell^2)} \leqslant \frac{4(1-3s_\ell^2c_\ell^2)}{3(1-3s_\ell^2c_\ell^2)} = \frac{4}{3}, \\ \frac{c_\ell^4}{1-3s_\ell^2c_\ell^2} = 1 + \frac{c_\ell^4 - 1 + 3s_\ell^2c_\ell^2}{1-3s_\ell^2c_\ell^2} &= 1 + \frac{-1 + c_\ell^2(c_\ell^2 + 3s_\ell^2)}{1-3s_\ell^2c_\ell^2} \\ = 1 + \frac{-1 + (1-s_\ell^2)(1+2s_\ell^2)}{1-3s_\ell^2c_\ell^2} &= 1 + \frac{s_\ell^2 \overbrace{(1-2s_\ell^2)}^{\geqslant 0}}{1-3s_\ell^2c_\ell^2} \geqslant 1\end{aligned} \tag{79}$$

because $s_\ell^2 \leqslant \frac{1}{2}$ for all $\ell = 1, \ldots, \bar{N}$.

- Finally, inequality (52) can be derived similarly by invoking

$$\begin{aligned}\zeta^{-1} s_\ell^2 c_\ell^2 \frac{d^{(N+1-\ell)}}{\bar{d}^{(\ell)}} &= \zeta^{-1} s_\ell^2 c_\ell^2 \frac{2c_\ell^2 d_{ii}}{2\zeta^{-1} s_\ell^2 c_\ell^2 d_{ii}} = c_\ell^2, \\ 0 \leqslant \zeta^{-1} s_\ell^2 c_\ell^2 \frac{2m^{(N+1-\ell)} - (1-2\theta)\tau d^{(N+1-\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}} &= c_\ell^2 \frac{2\zeta^{-1} s_\ell^2 m^{(N+1-\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}} \\ &\leqslant c_\ell^2 \frac{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}}{2\bar{m}^{(\ell)} - (1-2\theta)\tau\bar{d}^{(\ell)}} \leqslant c_\ell^2\end{aligned}$$

because $s_\ell^2 \leqslant \frac{1}{2} < 1$ for $\zeta = 1$ and

$$\zeta^{-1} s_\ell^2 m^{(N+1-\ell)} - \bar{m}^{(\ell)} = m_{ii}(3s_\ell^2 - 2s_\ell^2c_\ell^2 - 3 + 8s_\ell^2c_\ell^2) = m_{ii}(6s_\ell^2c_\ell^2 - 3c_\ell^2) = 3c_\ell^2 m_{ii}(2s_\ell^2 - 1) \leqslant 0$$

in case of a finite element approximation. □