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Robust Preconditioning for Space-Time Isogeometric Analysis of Parabolic Evolution Problems

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Abstract. We propose and investigate new robust preconditioners for space-time Isogeometric Analysis of parabolic evolution problems. These preconditioners are based on a time parallel multigrid method. We consider a decomposition of the space-time cylinder into time-slabs which are coupled via a discontinuous Galerkin technique. The time-slabs provide the structure for the time-parallel multigrid solver. The most important part of the multigrid method is the smoother. We utilize the special structure of the involved operator to decouple its application into several spatial problems by means of generalized eigenvalue or Schur decompositions. Some of these problems have a symmetric saddle point structure, for which we present robust preconditioners. Finally, we present numerical experiments confirming the robustness of our space-time IgA solver.

Key words: parabolic evolution problems, isogeometric analysis, discontinuous Galerkin, robust preconditioners, parallelization

1 Introduction

Time-dependent Partial Differential Equations (PDEs) of parabolic type play an important role in the simulation of various physical processes, like heat conduction, diffusion, and 2d eddy-current problems in electromagnetics. They are often given as initial-boundary value problems (IBVP). The discretization of such problems is usually performed either by first discretizing in time by a time-stepping method and then in space by, e.g., finite elements or vice versa. The former approach is often denoted as Rothe's method [22] and the latter one vertical method of lines [30]. Both of the two approaches are sequential in time. In order to treat such problems on massively parallel computers, different approaches are required to overcome the sequential structure. There exist various techniques for parallelization in time. We refer to [6] for an overview of time-parallel methods.

In the current work, we focus on space-time methods. More precisely, we consider the time as just another variable, say x_{d+1}, where $x_1, \ldots, x_d$ are the d-dimensional spatial variables. The derivative in time direction is then viewed as a strong convection term in the direction x_{d+1}. In order to provide a stable discretization, we use stabilization techniques developed for convection dominated elliptic convection-diffusion problems, see, e.g., [28]. To be more precise, we consider the Streamline-Upwind Petrov-Galerkin (SUPG) method, introduced

in [16]. We consider the linear parabolic IBVP, find $u : \overline{Q} \to \mathbb{R}$ such that

$$\partial_t u - \Delta u = f \text{ in } Q,\ u = 0 \text{ on } \Sigma, \text{ and } u = u_0 \text{ on } \overline{\Sigma}_0, \tag{1.1}$$

as a typical parabolic model problem posed in the space-time cylinder $\overline{Q} = \overline{\Omega} \times \overline{J} = \overline{\Omega} \times [0,T] = Q \cup \Sigma \cup \overline{\Sigma}_0 \cup \overline{\Sigma}_T$, where ∂_t denotes the partial time derivative, Δ is the Laplace operator, f is a given source function, u_0 are the given initial data, T is the final time, $J = (0,T)$ is the time interval, $Q = \Omega \times (0,T)$, $\Sigma = \partial\Omega \times (0,T)$, $\Sigma_0 := \Omega \times \{0\}$, $\Sigma_T := \Omega \times \{T\}$, and $\Omega \subset \mathbb{R}^d$ $(d = 1,2,3)$ denotes the spatial computational domain with the boundary $\partial\Omega$. In [23], a time-upwind test functions were used to construct a stable single-patch discretization scheme in the Isogeometric Analysis (IgA) framework. This approach was extended in [13] to multiple patches in time, where each space-time patch Q_n is given as space-time-slab $Q_n = \Omega \times (t_{n-1}, t_n)$ corresponding to a decomposition $0 = t_0 < t_1 < \ldots < t_N = T$ of the time interval $[0,T]$. A discontinuous Galerkin (dG) technique was used for coupling the space-time-slabs in an appropriate way. Finally, the resulting huge linear system $\mathbf{L}_h \mathbf{u}_h = \mathbf{f}_h$ is solved by the time-parallel multigrid (MG) method introduced in [7]. The main new contributions of this paper are the smoothers that finally yield a robust multigrid solver and preconditioner for the GMRES solver, respectively.

IgA is a powerful methodology for discretizing PDEs. It was first introduced in [17] and its advantages have been highlighted in many publications, see, e.g., the monograph [5], the survey paper [3] and the references therein. The main idea is to use that same smooth higher order splines for both representing the computational domain and approximating the solution of the PDE or the PDE system. The most common choices are B-Splines, Non-Uniform Rational B-Splines (NURBS), T-Splines, Truncated Hierarchical B-Splines (THB-Splines), etc., see, e.g., [8], [9] and [2]. One of the strengths of IgA is the capability of creating high-order spline spaces, while keeping the number of degrees of freedom quite small.

The purpose of this paper is to investigate the efficient realization of the time-parallel MG method mentioned above. The special time-multipatch dG structure of the discretization leads to a block-bidiagonal matrix $\mathbf{L}_h = \text{blockbidiag}(-\mathbf{B}_n, \mathbf{A}_n)$, where the block-diagonal matrices $\mathbf{A}_n$, $i = 1, \ldots, N$, and the block-subdiagonal matrices $\mathbf{B}_n$, $i = 2, \ldots, N$, have tensor product representations. The most costly part of the MG method is the application of the smoother, which is of (inexact) damped block Jacobi type, i.e,

$$u_h^{k+1} = u_h^k + \omega \mathbf{D}_h^{-1} \left[f_h - \mathbf{L}_h u_h^k \right] \quad \text{for } k = 1, 2, \ldots.$$

The block diagonal matrix $\mathbf{D}_h$ is formed by the diagonal blocks of $\mathbf{L}_h$, i.e., by $\mathbf{A}_n$. This paper investigates the efficient application of $\mathbf{A}_n^{-1}$ by utilizing its tensor product structure. We use ideas from [29] and [26] to perform a decomposition of $\mathbf{A}_n$ into a series of spatial problems, for which we investigate robust block preconditions. These preconditioners are constructed by means of operator interpolation, see, e.g., [33], [4] and [1]. Moreover, their application can be further accelerated by using domain decomposition or multigrid approaches in connection with parallelization in space.

The remainder of the paper is organized as follows. In Section 2, we rephrase basic definitions and the stable space-time dG-IgA variational formulation. Section 3 is devoted to the construction of efficient smoothers used in the time-parallel multigrid solver respectively preconditioner. Numerical experiments confirming the theoretical results are presented in Section 4. Finally, we draw some conclusions in Section 5.

2 Preliminaries

In this section, we introduce the IgA concept, recall some important definitions, and state the space-time variational IgA scheme derived and analysed in [13]. For a more detailed discussion of IgA, we refer to [5] and [3]. We follow the notation used in [13].

2.1 Isogeometric Analysis

Let $\hat{\Omega} := (0,1)^d$, be the d-dimensional unit cube, which we refer to as the *parameter domain*. Let p_ι and $N_\iota, \iota \in \{1,\dots,d\}$, denote the degree and the number of basis functions in x_ι-direction. Moreover, let $\Xi_\iota = \{\xi_1 = 0, \xi_2, \dots, \xi_{n_\iota} = 1\}$, $n_\iota = N_\iota - p_\iota - 1$, be a partition of $[0,1]$, called *knot vector*. With this ingredients we are able to define the B-Spline basis $\hat{N}_{i,p}$, $i \in \{1,\dots,N_\iota\}$ on $[0,1]$ via Cox-De Boor's algorithm, cf. [5]. The generalization to $\hat{\Omega}$ is realized by considering a tensor product, again denoted by $\hat{N}_{i,p}$, where $i = (i_1,\dots,i_d)$ and $p = (p_1,\dots,p_d)$ are a multi-indices. For notational simplicity, we define $\mathcal{I} := \{(i_1,\dots,i_d) \,|\, i_\iota \in \{1,\dots,N_\iota\}\}$ as the set of multi-indices.

The computational domain Ω, also called *physical domain*, is parametrized by the B-Spline basis functions. It is given as image of the parameter domain $\hat{\Omega}$ under the so-called *geometrical mapping* $G: \hat{\Omega} \to \mathbb{R}^d$, defined as

$$G(\xi) := \sum_{i \in \mathcal{I}} P_i \hat{N}_{i,p}(\xi),$$

with the control points $P_i \in \mathbb{R}^d$, $i \in \mathcal{I}$. In order to represent more complicated geometries Ω, multiple non-overlapping domains (patches) $\Omega_n := G_n(\hat{\Omega}), n = 1,\dots,N$ are composed, where each patch is associated with a different geometrical mapping G_n. In the following, we refer to such domains $\overline{\Omega} := \bigcup_{n=1}^N \overline{\Omega}_n$ as *multipatch domains*.

In the IgA concept, the B-Splines are not only used for representing the geometry, but also as basis for finite-dimensional space used for approximating the solution of the PDE. This motivates to define the basis functions $N_{i,p} := \hat{N}_{i,p} \circ G^{-1}$ in the physical space by mapping the corresponding basis functions $\hat{N}_{i,p}$ defined in the parameter domain $\hat{\Omega}$.

On each patch Ω_n, we now define the local IgA space

$$V_h^n := \operatorname{span}\{N_{i,p}\}_{i \in \mathcal{I}}. \tag{2.1}$$

The construction of global IgA space V_h depends on the used formulation, and is given in the next section.

2.2 Space-time variational formulation and its IgA discretization

Let Ω be a bounded Lipschitz domain in $\mathbb{R}^d$, $d = 1, 2$, or 3, with the boundary $\Gamma = \partial\Omega$. For any multi-index $\boldsymbol{\alpha} = (\alpha_1,\dots,\alpha_d)$ of non-negative integers $\alpha_1,\dots,\alpha_d$, we define the differential operator $\partial_x^{\boldsymbol{\alpha}} = \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d}$, with $\partial_{x_j} = \partial/\partial x_j$, $j = 1,\dots,d$. As usual, $L_2(\Omega)$ denotes the Lebesgue space of all Lebesgue measurable and square-integrable functions endowed with the norm $\|v\|_{L_2(\Omega)} = \left(\int_\Omega |v(x)|^2\,dx\right)^{0.5}$, and $L_\infty(\Omega)$ denotes the space of

functions that are essentially bounded. For a non-negative integer ℓ, we define the standard Sobolev space

$$H^\ell(\Omega) = \{v \in L_2(\Omega) : \partial_x^{\boldsymbol{\alpha}} v \in L_2(\Omega) \text{ for all } |\boldsymbol{\alpha}| = \textstyle\sum_{j=1}^d \alpha_j \le \ell\},$$

endowed with the norm

$$\|v\|_{H^\ell(\Omega)} = \big(\sum_{0\le|\boldsymbol{\alpha}|\le\ell} \|\partial_x^{\boldsymbol{\alpha}} v\|^2_{L_2(\Omega)}\big)^{\frac{1}{2}},$$

whereas the trace space of $H^1(\Omega)$ is denoted by $H^{\frac{1}{2}}(\Gamma)$. Further, we introduce the subspace $H_0^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma\}$ of all functions v from $H^1(\Omega)$ with zero traces on Γ. We define the spatial gradient by $\nabla_x v = (\partial_{x_1} v, \dots, \partial_{x_d} v)$. Let ℓ and m be positive integers. For functions defined in the space-time cylinder Q, we define the Sobolev spaces

$$H^{\ell,m}(Q) = \{v \in L_2(Q) : \partial_x^{\boldsymbol{\alpha}} v \in L_2(Q) \text{ for } 0 \le |\boldsymbol{\alpha}| \le \ell, \text{ and } \partial_t^i v \in L_2(Q),\ i = 1, \dots, m\},$$

where $\partial_t = \partial/\partial t$, and, in particular, the subspaces

$$\begin{aligned} H_0^{1,0}(Q) =& \{v \in L_2(Q) : \nabla_x v \in [L_2(Q)]^d,\ v = 0 \text{ on } \Sigma\} \text{ and} \\ H_{0,\bar{0}}^{1,1}(Q) =& \{v \in L_2(Q) : \nabla_x v \in [L_2(Q)]^d,\ \partial_t v \in L_2(Q), v = 0 \text{ on } \Sigma,\ v = 0 \text{ on } \Sigma_T\}. \end{aligned}$$

We equip the above spaces with the norms and seminorms

$$\|v\|_{H^{\ell,m}(Q)} = \big(\sum_{|\boldsymbol{\alpha}|\le\ell} \|\partial_x^{(\alpha_1,\dots,\alpha_d)} v\|^2_{L_2(Q)} + \sum_{m_0=0}^{m} \|\partial_t^{m_0} v\|^2_{L_2(Q)}\big)^{\frac{1}{2}}$$

and

$$|v|_{H^{\ell,m}(Q)} = \big(\sum_{|\boldsymbol{\alpha}|=\ell} \|\partial_x^{(\alpha_1,\dots,\alpha_d)} v\|^2_{L_2(Q)} + \|\partial_t^{m} v\|^2_{L_2(Q)}\big)^{\frac{1}{2}},$$

respectively.

Using the standard procedure and integration by parts with respect to both x and t, we can easily derive the following space-time variational formulation of (1.1): find $u \in H_0^{1,0}(Q)$ such that

$$a(u, v) = l(v) \quad \text{for all } v \in H_{0,\bar{0}}^{1,1}(Q), \tag{2.2}$$

with the bilinear form

$$a(u, v) = -\int_Q u(x,t)\partial_t v(x,t)\,dx\,dt + \int_Q \nabla_x u(x,t) \cdot \nabla_x v(x,t)\,dx\,dt$$

and the linear form

$$l(v) = \int_Q f(x,t)v(x,t)\,dx\,dt + \int_\Omega u_0(x)v(x,0)\,dx,$$

where the source $f \in L_2(Q)$ and the initial conditions $u_0 \in L_2(\Omega)$ are given.

Without loss of generality, we only consider homogeneous Dirichlet boundary conditions on Σ. The method presented in this paper can easily be generalized to other constellations of boundary conditions. The space-time variational formulation (2.2) has a unique solution, see, e.g, [20] and [21].

Assumption 1 *We assume that the solution u of (2.2) belongs to $V = H_0^{1,0}(Q) \cap H^{\ell,m}(Q)$ with some $\ell \geq 2$ and $m \geq 1$.*

We describe the space-time cylinder Q as a union of non-overlapping time slabs Q_1, Q_2,...,Q_N. We consider a partition $0 = t_0 < t_1 < \ldots < t_N = T$ of the time interval $[0, T]$, and denote the sub intervals by $J_n = (t_{n-1}, t_n)$. We now define the time slabs $Q_n = \Omega \times J_n$ and the faces $\Sigma_n = \overline{Q}_{n+1} \cap \overline{Q}_n = \Omega \times \{t_n\}$ between the time slabs, where we identify Σ_T and Σ_N. In that way, we have the decomposition $\overline{Q} = \cup_{n=1}^N \overline{Q}_n$, where each space-time cylinder Q_n has a geometrical mapping G_n. To keep the notation simple, in what follows, we will use the sup-index n to denote the restrictions to Q_n, e.g., $u^n := u|_{Q_n}$.

Remark 2.1. We note that the spatial domain Ω can also be a multipatch domain. This leads to a representation of Q_n as union of non-overlapping space-time patches $Q_{n,k}, k = 1, \ldots, K$, i.e., $\overline{Q}_n = \cup_{k=1}^K \overline{Q}_{n,k}$. The corresponding bases are then coupled in a conforming way.

We denote the global discontinuous B-Spline space and the local continuous patch-wise B-Spline spaces by

$$V_{0h} = \{v_h \in L_2(Q) : v_h|_{Q_n} \in V_h^n, \text{ for } n = 1, \ldots, N, \text{ and } v_h|_\Sigma = 0\} \tag{2.3}$$

and

$$V_{0h}^n = \{v_h \in V_h^n, \text{ for } n = 1, \ldots, N, \text{ and } v_h|_\Sigma = 0\}, \tag{2.4}$$

respectively. Notice that $v_h \in V_{0h}$ is discontinuous across Σ_n. We introduce the notations

$$v_{h,+}^n = \lim_{\varepsilon \to 0^+} v_h(t_n + \varepsilon),\ v_{h,-}^n = \lim_{\varepsilon \to 0^-} v_h(t_n + \varepsilon),\ [\![v_h]\!]^n = v_{h,+}^n - v_{h,-}^n,\ [\![v_h]\!]^0 = v_{h,+}^0,$$

where $[\![v_h]\!]^n$ denotes the jump of v_h across Σ_n for $n \geq 1$, and $[\![v_h]\!]^0 = v_{h,+}^0$ denotes the trace of v_h on Σ_0. For a smooth function u, we obviously have $[\![u]\!]^n = u_+^n - u_-^n = 0$ for $n \geq 1$, and $[\![u]\!]^0 = u|_{\Sigma_0}$.

Let us now consider the space-time slab Q_n, and let us denote the outer normal to ∂Q_n by $\mathbf{n} = (n_1, \ldots, n_d, n_{d+1}) = (\mathbf{n}_x, n_t)$. For the time being, we assume that u^{n-1} is known. Let $v_h^n \in V_{0h}^n$ and $w_h^n = v_h^n + \theta_n\, h_n \partial_t v_h^n$ with some positive parameter θ_n, which will be defined later. We note that $w_h^n\big|_\Sigma = 0$. Multiplying $\partial_t u - \Delta u = f$ by w_h^n, integrating over Q_n, and applying integration by parts, we arrive at the variational identity

$$\begin{aligned}
&\int_{Q_n} (\partial_t u\, (v_h^n + \theta_n\, h_n \partial_t v_h^n) + \nabla_x u \cdot \nabla_x v_h^n + \theta_n\, h_n \nabla_x u \cdot \nabla_x \partial_t v_h^n)\, dx\, dt \\
&- \int_{\partial Q_n} n_x \cdot \nabla_x u (v_h^n + \theta_n\, h_n \partial_t v_h^n)\, dx + \int_{\Sigma_{n-1}} u_+^{n-1}\, v_{h,+}^{n-1}\, dx \\
&= \int_{Q_n} f\, (v_h^n + \theta_n\, h_n \partial_t v_h^n)\, dx\, dt + \int_{\Sigma_{n-1}} u_-^{n-1}\, v_{h,+}^{n-1}\, dx
\end{aligned}$$

for $n = 1, \ldots, N$, where we used that $u_-^{n-1} = u_+^{n-1} = u^{n-1}$ on every Σ_{n-1}. Furthermore, using $n_x|_{\Sigma_n} = 0$ and $w_h = 0$ on Σ, we have

$$\begin{aligned}
a_{Q_n}(u, v_h) := &\int_{Q_n} (\partial_t u\, (v_h^n + \theta_n\, h_n \partial_t v_h^n) + \nabla_x u \cdot \nabla_x v_h^n + \theta_n\, h_n \nabla_x u \cdot \nabla_x \partial_t v_h^n)\, dx\, dt \\
&+ \int_{\Sigma_{n-1}} [\![u]\!]^{n-1}\, v_{h,+}^{n-1}\, dx = \int_{Q_n} f\, (v_h^n + \theta_n\, h_n \partial_t v_h^n)\, dx\, dt,
\end{aligned}$$

for all $n = 2, \ldots, N$, and

$$a_{Q_1}(u, v_h) := \int_{Q_1} (\partial_t u\,(v_h^1 + \theta_1\, h_1 \partial_t v_h^1) + \nabla_x u \cdot \nabla_x v_h^1 + \theta_1\, h_1 \nabla_x u \cdot \nabla_x \partial_t v_h^1)\, dx\, dt$$
$$+ \int_{\Sigma_0} [\![u]\!]^0\, v_{h,+}^0\, dx = \int_{Q_1} f\,(v_h^1 + \theta_1\, h_1 \partial_t v_h^1)\, dx\, dt + \int_{\Sigma_0} u_0\, v_{h,+}^0\, dx.$$

Summing over all Q_n, we conclude that

$$a_h(u, v_h) = l_h(v_h), \quad \forall v_h \in V_{0h}, \tag{2.5}$$

where

$$a_h(u, v_h) = \sum_{n=1}^{N} a_{Q_n}(u, v_h)$$

and

$$l_h(v_h) = \sum_{n=1}^{N} \int_{Q_n} f\,(v_h^n + \theta_n\, h_n \partial_t v_h^n)\, dx\, dt + \int_{\Sigma_0} u_0\, v_{h,+}^0\, dx.$$

Now, the space-time dG IgA variational scheme for (1.1) reads as follows: Find $u_h \in V_{0h}$ such that

$$a_h(u_h, v_h) = l_h(v_h), \quad \forall v_h \in V_{0h}. \tag{2.6}$$

Motivated by the definition of the bilinear form $a_h(\cdot, \cdot)$ in (2.6), we introduce the mesh-dependent dG norm

$$\|v\|_{dG} := \Big(\sum_{n=1}^{N} \Big(\|\nabla_x v\|_{L_2(Q_n)}^2 + \theta_n\, h_n\, \|\partial_t v\|_{L_2(Q_n)}^2 + \frac{1}{2} \|[\![v]\!]^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \Big) + \frac{1}{2} \|v\|_{L_2(\Sigma_N)}^2 \Big)^{\frac{1}{2}},$$

In the following, we recall some important properties of the IgA scheme (2.6) respectively the bilinear form $a_h(\cdot, \cdot)$. For the proofs, we refer to [13].

Lemma 2.1. *The bilinear form $a_h(\cdot, \cdot)$, defined in (2.6), is V_{0h}-elliptic, i.e.,*

$$a_h(v_h, v_h) \geq C_e \|v_h\|_{dG}^2, \quad \text{for } v_h \in V_{0h}, \tag{2.7}$$

where $C_e = 0.5$ for $\theta_n \leq C_{inv,0}^{-2}$, with the positive, h_n-independent constant $C_{inv,0}$ from the inverse inequality

$$\|v_h\|_{L_2(\Sigma_{n-1})}^2 \leq C_{inv,0} h_n^{-1} \|v_h\|_{L_2(Q_n)}^2$$

that holds for all $v_h \in V_h^n$, $n = 1, \ldots, N$.

The V_{0h}-ellipticity of the bilinear form $a_h(\cdot, \cdot)$ implies that there exists a unique solution to (2.5). In order to obtain a priori error estimates, we introduce the space $V_{0h,*} = V + V_{0h}$ endowed with the norm

$$\|v\|_{dG,*} := \Big(\|v\|_{dG}^2 + \sum_{n=1}^{N} (\theta_n h_n)^{-1} \|v\|_{L_2(Q_n)}^2 + \sum_{n=2}^{N} \|v_-^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \Big)^{\frac{1}{2}}. \tag{2.8}$$

Lemma 2.2. *Let $u \in V_{0h,*}$. Then the boundedness inequality*

$$|a_h(u, v_h)| \leq C_b \|u\|_{dG,*} \|v_h\|_{dG} \tag{2.9}$$

holds for all $v_h \in V_{0h}$, where $C_b = \max(C_{inv,1}\, \theta_{max}, 2)$, with $\theta_{max} = \max_n\{\theta_n\} \leq C_{inv,0}^{-2}$ and the positive, h_n-independent constant $C_{inv,1}$ from the inverse inequality

$$\|\partial_t \partial_{x_i} v_h\|^2_{L_2(Q_n)} \leq C_{inv,1} h_n^{-2} \|\partial_{x_i} v_h\|^2_{L_2(Q_n)}$$

that holds for all $v_h \in V_h^n$, $n = 1, \ldots, N$, $i = 1, \ldots, n$.

Theorem 2.1. *Let u and u_h solve (2.2) and (2.6), respectively. Under the regularity Assumption 1, there exists a positive generic constant C, which is independent of $h = \max\{h_n\}$, such that*

$$\|u - u_h\|_{dG} \leq C(h^{\ell-1} + h^{m-\frac{1}{2}})\, \|u\|_{H^{\ell,m}(Q)}. \tag{2.10}$$

Moreover, if $1 \leq m < \ell \leq p+1$, then

$$\|u - u_h\|_{dG} \leq C h^{m-\frac{1}{2}} \|u\|_{H^{\ell,m}(Q)}. \tag{2.11}$$

Remark 2.2. We remark that, for the case of highly smooth solutions, i.e., $p + 1 \leq \min(\ell, m)$, estimate (2.10) takes the form

$$\|u - u_h\|_{dG} \leq C\, h^p\, \|u\|_{H^{\ell,m}(Q)}. \tag{2.12}$$

2.3 Efficient Matrix Assembly

Let us recall the IgA variational problem given in (2.6). The local bilinear form for each space-time slab Q_n is given by

$$\begin{aligned} a_{Q_n}(u_h, v_h) = &\int_{Q_n} \partial_t\, u_h^n\, (v_h^n + \theta_n\, h_n \partial_t v_h^n) + \nabla_x\, u_h^n \cdot \nabla_x (v_h^n + \theta_n\, h_n \partial_t v_h^n)\, dx\, dt \\ &+ \int_{\Sigma_{n-1}} u_{h,+}^{n-1}\, v_{h,+}^{n-1}\, ds - \int_{\Sigma_{n-1}} u_{h,-}^{n-1}\, v_{h,+}^{n-1}\, ds \\ =:& b_{Q_n}(u_h^n, v_h^n) - \int_{\Sigma_{n-1}} u_{h,-}^{n-1}\, v_{h,+}^{n-1}\, ds, \end{aligned}$$

where $n = 1, \ldots, N$. For the local spaces V_{0h}^n defined by (2.4), we now introduce the simpler notation φ_j^n for the B-Spline basis functions such that

$$V_{0h}^n = \operatorname{span}\{\varphi_j^n\}_{j=1}^{N_n}$$

for $n = 1, \ldots, N$. Once the basis is chosen, from the IgA variational scheme (2.6), we immediately obtain the linear system

$$\mathbf{L}_h \boldsymbol{u}_h := \begin{pmatrix} \mathbf{A}_1 & & & \\ -\mathbf{B}_2\, \mathbf{A}_2 & & & \\ & \ddots & \ddots & \\ & & -\mathbf{B}_N\, \mathbf{A}_N \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{u}_N \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \\ \vdots \\ \boldsymbol{f}_N \end{pmatrix} =: \boldsymbol{f}_h, \tag{2.13}$$

with the matrices

$$\mathbf{A}_n[i,j] := b_{Q_n}(\varphi_j^n, \varphi_i^n) \quad \text{for } i,j = 1,\dots,N_n$$

on the diagonal for $n = 1,\dots,N$, and the matrices

$$\mathbf{B}_n[i,k] := \int_{\Sigma_{n-1}} \varphi_{k,-}^{n-1}\, \varphi_{i,+}^{n-1}\, ds \quad \text{for } k = 1,\dots,N_{n-1} \text{ and } i = 1,\dots,N_n.$$

on the lower off diagonal for $n = 2,\dots,N$. Moreover, the right hand sides are given by

$$\boldsymbol{f}_n[i] := l_h(\varphi_i^n), \quad i = 1,\dots,N_n,$$

for $n = 1,\dots,N$.

If the geometrical mappings $G_n : \widehat{Q} \to Q_n, n = 1,\dots,N$, preserve the tensor product structure of the IgA basis functions φ_i^n, we can use this information to save assembling time and storage costs for the linear system (2.13). In this case, we can write the basis functions φ_i^n in the form

$$\varphi_i^n(x,t) = \phi_{i_x}^n(x)\psi_{i_t}^n(t) \quad \text{with } i_x \in \{1,\dots,N_{n,x}\} \text{ and } i_t \in \{1,\dots,N_{n,t}\},$$

where $N_n = N_{n,x}N_{n,t}$. Using this representation, we can write the matrices $\mathbf{A}_n, n = 1,\dots,N$ as

$$\mathbf{A}_n = \mathbf{K}_{n,t} \otimes \mathbf{M}_{n,x} + \mathbf{M}_{n,t} \otimes \mathbf{K}_{n,x}, \tag{2.14}$$

with the standard mass and stiffness matrices with respect to space

$$\mathbf{M}_{n,x}[i_x,j_x] := \int_\Omega \phi_{j_x}^n \phi_{i_x}^n\, dx, \qquad \mathbf{K}_{n,x}[i_x,j_x] := \int_\Omega \nabla_x \phi_{j_x}^n \cdot \nabla_x \phi_{i_x}^n\, dx,$$

where $i_x, j_x = 1,\dots,N_{n,x}$, and corresponding matrices with respect to time

$$\begin{aligned} \mathbf{K}_{n,t}[i_t,j_t] &:= \int_{t_{n-1}}^{t_n} \partial_t \psi_{j_t}^n (\psi_{i_t}^n + \theta_n h_n \partial_t \psi_{i_t}^n)\, dt + \psi_{j_t}^n(t_{n-1})\psi_{i_t}^n(t_{n-1}), \\ \mathbf{M}_{n,t}[i_t,j_t] &:= \int_{t_{n-1}}^{t_n} \psi_{j_t}^n (\psi_{i_t}^n + \theta_n h_n \partial_t \psi_{i_t}^n)\, dt, \end{aligned} \tag{2.15}$$

with $i_t, j_t = 1,\dots,N_{n,t}$. The matrices on the off diagonal $\mathbf{B}_n, n = 2,\dots,N$, can be written in the form

$$\mathbf{B}_n := \mathbf{N}_{n,t} \otimes \widetilde{\mathbf{M}}_{n,x},$$

with the matrices

$$\widetilde{\mathbf{M}}_{n,x}[i_x,k_x] := \int_\Omega \phi_{k_x}^{n-1}\phi_{i_x}^n\, dx \quad \text{and} \quad \mathbf{N}_{n,t}[i_t,k_t] := \psi_{k_t}^{n-1}(t_{n-1})\psi_{i_t}^n(t_{n-1}),$$

where $i_x = 1,\dots,N_{n,x}$, $k_x = 1,\dots,N_{n-1,x}$, $i_t = 1,\dots,N_{n,t}$ and $k_t = 1,\dots,N_{n-1,t}$.

3 Solvers for space-time problems

This section aims at the development of an efficient solver for the huge space-time system (2.13). Our new solver is based on the time parallel multigrid method proposed in [7], see also the PhD thesis [25]. The key point in realizing the method efficiently is the application of the smoother, which is the most costly part of the algorithm. The goal is to utilize the structure of the involved matrix $\mathbf{A}_n^{-1}$, which then allows for a faster application.

3.1 Time-parallel multigrid

We want to give an overview of the time-parallel multigrid method introduced in [25]. Multigrid consists of three main ingredients: the coarse grid solver, the smoother and the prolongation/restriction operators. Concerning the restriction and prolongation operator, it is advantageous to consider coarsening in space and in time separately. The restriction in time direction is realized by combining two consecutive time-slabs into a single one. For a more detailed discussion on how space and time coarsening can be combined, we refer to [25].

In this work, we are mostly interested in the smoother, which is of (inexact) damped block Jacobi type, i.e.,

$$u_h^{k+1} = u_h^k + \omega \mathbf{D}_h^{-1} \left[f_h - \mathbf{L}_h u_h^k \right] \quad \text{for } k = 1, 2, \dots .$$

We use the block diagonal matrix $\mathbf{D}_h := \operatorname{diag}\{\mathbf{A}_n\}_{n=1}^N$ and the damping parameter $\omega = \frac{1}{2}$, see also [7]. The application of the smoother can be accelerated by replacing the inverse of $\mathbf{D}_h$ by some approximation, i.e., an approximation $\hat{\mathbf{A}}_n^{-1}$ to $\mathbf{A}_n^{-1}$. The aim of this work is to find a procedure, which allows an efficient application of $\hat{\mathbf{A}}_n^{-1}$ to a vector. In order to achieve this, we will heavily exploiting the special tensor structure of $\mathbf{A}_n$.

3.2 General construction of an approximation for $\mathbf{A}_n^{-1}$

In this section, for notational simplicity, we drop the subscript n when considering matrices and vectors defined on the space-time slice Q_n. We recall the structure of the matrix $\mathbf{A}$,

$$\mathbf{A} = \mathbf{K}_t \otimes \mathbf{M}_x + \mathbf{M}_t \otimes \mathbf{K}_x,$$

where the matrices $\mathbf{M}_x$ and $\mathbf{K}_x$ are symmetric and positive definite, while the matrices $\mathbf{K}_t$ and $\mathbf{M}_t$ are non-symmetric, cf. (2.14). The matrices $\mathbf{M}_x$ and $\mathbf{K}_x$ correspond to d-dimensional problem, whereas $\mathbf{K}_t$ and $\mathbf{M}_t$ are only related to a one dimensional problem in one time-slice. Hence, the size of the latter two matrices is much smaller than the first two. The idea is to use already available preconditioners for symmetric positive definite problems of the form $\mathbf{K}_x + \gamma \mathbf{M}_x$ with $\gamma > 0$ to construct efficient and robust preconditioners for $\mathbf{A}^{-1}$. The ideas of this section are based on the results developed in [29] and [26].

We will achieve this by performing a decomposition of $\mathbf{M}_t^{-1}\mathbf{K}_t$ using one of the three following methods: *Diagonalization*, *Complex-Schur decomposition*, *Real-Schur decomposition*. We obtain a decomposition of the form $\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{X}^{-1}\mathbf{Z}\mathbf{X}$, where the entries of the matrices $\mathbf{X}$ and $\mathbf{Z}$ are complex or real numbers, and $\mathbf{Z}$ has some sort of "simple" structure. A detailed specification will be presented in Section 3.3, Section 3.4 and Section 3.5.

By defining $\mathbf{Y} := (\mathbf{M}_t\mathbf{X})^{-1}$, we obtain the following representations

$$\mathbf{M}_t = \mathbf{Y}^{-1}\mathbf{X}^{-1} \quad \text{and} \quad \mathbf{K}_t = \mathbf{Y}^{-1}\mathbf{Z}\mathbf{X}^{-1}.$$

Now we can rewrite $\mathbf{A}$ in the form

$$\begin{aligned}
\mathbf{A} &= \mathbf{K}_t \otimes \mathbf{M}_x + \mathbf{M}_t \otimes \mathbf{K}_x \\
&= (\mathbf{Y}^{-1}\mathbf{Z}\mathbf{X}^{-1}) \otimes \mathbf{M}_x + (\mathbf{Y}^{-1}\mathbf{X}^{-1}) \otimes \mathbf{K}_x \\
&= (\mathbf{Y}^{-1} \otimes \mathbf{I}) \cdot (\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x) \cdot (\mathbf{X}^{-1} \otimes \mathbf{I}).
\end{aligned}$$

Using the well-known fact that $(\mathbf{Y}^{-1} \otimes \mathbf{I})^{-1} = \mathbf{Y} \otimes \mathbf{I}$ and $(\mathbf{X}^{-1} \otimes \mathbf{I})^{-1} = \mathbf{X} \otimes \mathbf{I}$, we obtain

$$\mathbf{A}^{-1} = (\mathbf{X} \otimes \mathbf{I}) \cdot (\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} \cdot (\mathbf{Y} \otimes \mathbf{I}). \tag{3.1}$$

In the subsequent subsections, we will investigate the structure of the matrix $(\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)$ for each of the decomposition methods, and we will look for efficient ways of (approximate) inversion.

In the following, the generalized eigenvalues $\lambda_i := \alpha_i + \imath\beta_i \in \mathbb{C}$ of $(\mathbf{K}_t, \mathbf{M}_t)$, i.e.,

$$\mathbf{K}_t \mathbf{z}_i = \lambda_i \mathbf{M}_t \mathbf{z}_i, \tag{3.2}$$

with the eigenvector $\mathbf{z} := \mathbf{x} + \imath\mathbf{y}$, will play an important role for constructing an efficient application of (3.1). First of all, for $0 < \theta_n \leq C_{inv}^{-2}$, where C_{inv} denotes the constant from the inverse inequality

$$|v(t_{n-1})|^2 \leq C_{inv}^2 h_n^{-1} \|v\|^2_{L_2(t_{n-1},t_n)} \; \forall v \leftrightarrow \mathbf{v} \in \mathbb{R}^{N_t}, \tag{3.3}$$

we have the positiveness of the matrices $\mathbf{K}_t$ and $\mathbf{M}_t$, see [31] for an explicit formula of $C_{inv} = C_{inv}(p)$ in the case of polynomials of the degree p.

Lemma 3.1. *Let $\mathbf{K}_t$ and $\mathbf{M}_t$ be given by (2.15), and let the constant $C_{inv} > 0$ be defined according to (3.3). If $\theta_n > 0$, then the matrix $\mathbf{K}_t$ is positive, i.e., $\mathbf{v}^T \mathbf{K}_t \mathbf{v} > 0$ for all $\mathbf{v} \in \mathbb{R}^{N_t} \setminus \{\mathbf{0}\}$, and if $\theta_n < 2C_{inv}^{-2}$, then the matrix $\mathbf{M}_t$ is positive.*

Proof. We first consider the matrix $\mathbf{K}_t$. We can write $\mathbf{v}^T \mathbf{K}_t \mathbf{v}$ in the following way:

$$\begin{aligned}
\mathbf{v}^T \mathbf{K}_t \mathbf{v} = (\mathbf{K}_t \mathbf{v}, \mathbf{v}) &= \int_{t_{n-1}}^{t_n} (v'(t)v(t) + \theta_n h_n (v'(t))^2)\, dt + |v(t_{n-1})|^2 \\
&= \theta_n h_n \|v'\|^2_{L_2(t_{n-1},t_n)} + \frac{1}{2} \int_{t_{n-1}}^{t_n} (v^2)'(t)\, dt + |v(t_{n-1})|^2 \\
&= \theta_n h_n \|v'\|^2_{L_2(t_{n-1},t_n)} + \frac{1}{2}|v(t_n)|^2 - \frac{1}{2}|v(t_{n-1})|^2 + |v(t_{n-1})|^2 \\
&= \theta_n h_n \|v'\|^2_{L_2(t_{n-1},t_n)} + \frac{1}{2}(|v(t_n)|^2 + |v(t_{n-1})|^2) > 0.
\end{aligned}$$

for all $v \leftrightarrow \mathbf{v} \in \mathbb{R}^{N_t} \setminus \{\mathbf{0}\}$. Using (3.3), we similarly obtain

$$\begin{aligned}
\mathbf{v}^T \mathbf{M}_t \mathbf{v} = (\mathbf{M}_t \mathbf{v}, \mathbf{v}) &= \int_{t_{n-1}}^{t_n} (v(t)^2 + \theta_n h_n v'(t)v(t))\, dt \\
&= \|v\|^2_{L_2(t_{n-1},t_n)} + \frac{1}{2}\theta_n h_n (|v(t_n)|^2 - |v(t_{n-1})|^2) \\
&\geq \left(1 - \frac{C_{inv}^2 \theta_n}{2}\right) \|v\|^2_{L_2(t_{n-1},t_n)} + \frac{1}{2}\theta_n h_n |v(t_n)|^2 > 0.
\end{aligned}$$

for all $v \leftrightarrow \mathbf{v} \in \mathbb{R}^{N_t} \setminus \{\mathbf{0}\}$. □

Next we are going to investigate the generalized eigenvalues in (3.2). More precisely, we want to find conditions under which the real part α is positive. However, for a generalized eigenvalue problem $\mathbf{Az} = \lambda\mathbf{Bz}$, this does not follow from the positivity of $\mathbf{A}$ and $\mathbf{B}$ as following example shows.

Example 1. Let the matrices $\mathbf{A}$ and $\mathbf{B}$ be given by

$$\mathbf{A} = \begin{bmatrix} 5 & -2 \\ 13 & 18 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 4 & 10 \\ -10 & 9 \end{bmatrix}.$$

For the spectra, we have $\sigma(\mathbf{A}) = \{9 \pm 2\sqrt{5}\imath\}$ and $\sigma(\mathbf{B}) = \{\frac{13}{2} \pm 5\sqrt{15}\imath\}$. However, the generalized eigenvalues are $\sigma(\mathbf{B}^{-1}\mathbf{A}) = \{-\frac{103}{272} \pm \sqrt{4435}\imath\}$.

Let $\mathbf{z}$ be the eigenvector to the eigenvalue $\lambda = \alpha + \imath\beta$, i.e., $(\mathbf{A} - \lambda\mathbf{B})\mathbf{z} = 0$. Multiplying from the left with $(\mathbf{x} - \imath\mathbf{y})^T$ yields

$$(\mathbf{x} - \imath\mathbf{y})^T(\mathbf{A} - (\alpha + \imath\beta)\mathbf{B})(\mathbf{x} + \imath\mathbf{y}) = 0.$$

Separating the real and imaginary part, we obtain

$$\begin{aligned} \alpha(\mathbf{x}^T\mathbf{B}\mathbf{x} + \mathbf{y}^T\mathbf{B}\mathbf{y}) - \beta(\mathbf{x}^T(\mathbf{B} - \mathbf{B}^T)\mathbf{y}) &= \mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{y}^T\mathbf{A}\mathbf{y} \\ \alpha(\mathbf{x}^T(\mathbf{B} - \mathbf{B}^T)\mathbf{y}) + \beta(\mathbf{x}^T\mathbf{B}\mathbf{x} + \mathbf{y}^T\mathbf{B}\mathbf{y}) &= \mathbf{x}^T(\mathbf{A} - \mathbf{A}^T)\mathbf{y}. \end{aligned} \tag{3.4}$$

Introducing the abbreviations $a := \mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{y}^T\mathbf{A}\mathbf{y}$, $b := \mathbf{x}^T\mathbf{B}\mathbf{x} + \mathbf{y}^T\mathbf{B}\mathbf{y}$, $c := \mathbf{x}^T(\mathbf{B} - \mathbf{B}^T)\mathbf{y}$ and $d := \mathbf{x}^T(\mathbf{A} - \mathbf{A}^T)\mathbf{y}$, we can rewrite this system in the compact form

$$\begin{bmatrix} b & -c \\ c & b \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} a \\ d \end{bmatrix},$$

and α is then given by the formula

$$\alpha = \frac{1}{b^2 + c^2}(ab + cd). \tag{3.5}$$

We can easily observe the statements of the following lemma.

Lemma 3.2. *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be positive matrices, then the following statements hold:*

1. $a > 0$ *and* $b > 0$
2. *If* $\beta = 0$, *i.e., the eigenvalue* $\lambda \in \mathbb{R}$, *then* $\lambda = \alpha > 0$.
3. *If either* $\mathbf{A}$ *or* $\mathbf{B}$ *are symmetric, then* $\alpha > 0$.

If $\mathbf{A}$ *is only non-negative, then these inequalities hold with* $\geq$ *instead of* $>$.

Proof. The positivity of a and b immediately follows from the definition. If the eigenvalue λ is real, i.e., $\beta = 0$, we obtain from the first equation of (3.4) that $\alpha = a/b > 0$. If either $\mathbf{A}$ or $\mathbf{B}$ is symmetric, then either d or c is zero. Hence, by (3.5), α is positive. □

Let us now consider the special case of $\mathbf{A} = \mathbf{K}_t$ and $\mathbf{B} = \mathbf{M}_t$. For notational simplicity, we drop the subscript n, and consider the interval $[0, T]$. First we observe that

$$\begin{aligned} c = \mathbf{x}^T(\mathbf{B} - \mathbf{B}^T)\mathbf{y} &= \theta h \int_0^T y'(t)x(t) - x'(t)y(t)\,dt \\ d = \mathbf{x}^T(\mathbf{A} - \mathbf{A}^T)\mathbf{y} &= \int_0^T x'(t)y(t) - y'(t)x(t)\,dt. \end{aligned}$$

Hence, it follows that $c = -\theta h d$. This relation leads to the following formula for α:

$$\alpha = \frac{1}{b^2 + c^2}(ab - \theta h d^2). \tag{3.6}$$

The problem then reduces to check the relation $ab - \theta h d^2 > 0$, which then reads as

$$(\mathbf{x}^T \mathbf{A}\mathbf{x} + \mathbf{y}^T \mathbf{A}\mathbf{y})(\mathbf{x}^T \mathbf{B}\mathbf{x} + \mathbf{y}^T \mathbf{B}\mathbf{y}) - \theta h (x^T(\mathbf{A} - \mathbf{A}^T)\mathbf{y})^2 > 0, \tag{3.7}$$

for the eigenvector $\mathbf{z} = \mathbf{x} + \imath\mathbf{y}$ corresponding to $\lambda = \alpha + \imath\beta$. Rewriting (3.7) in terms of functions, we get the relation

$$\begin{aligned}
&\left(\theta_n h_n \|x'\|^2 + \frac{1}{2}(|x(T)|^2 + |x(0)|^2) + \theta_n h_n \|y'\|^2 + \frac{1}{2}(|y(T)|^2 + |y(0)|^2)\right) \\
&\cdot \left(\|x\|^2 + \frac{1}{2}\theta_n h_n (|x(T)|^2 - |x(0)|^2) + \|y\|^2 + \frac{1}{2}\theta_n h_n (|y(T)|^2 - |y(0)|^2)\right) \\
&- \theta h \left(\int_0^T x'(t)y(t) - y'(t)x(t)\, dt\right)^2 > 0
\end{aligned}$$

Unfortunately, in this work, we cannot give a complete characterization of the conditions under which the last inequality holds.

Let us consider the special case $\theta = 0$. First of all, we note that $\mathbf{v}^T \mathbf{K}_t \mathbf{v} = \frac{1}{2}(|v(t_{n-1})|^2 + |v(t_n)|^2)$, which then only defines a seminorm. Hence, discrete coercivity is not valid. Therefore, this case is not covered by the analysis presented in [13]. For its analysis, we refer to [27], where an inf-sup condition and error estimates are proven. The matrix $\mathbf{M}_t$ is symmetric and $\mathbf{v}^T \mathbf{M}_t \mathbf{v} = \|v\|_{L^2}^2$. From this fact, we can deduce the following statement by means of Lemma 3.2:

Proposition 3.1. *Let $\mathbf{K}_t$ and $\mathbf{M}_t$ be as defined above with $\theta = 0$. Then $\alpha \geq 0$.*

Remark 3.1. In the condition number analysis of the following subsections, we consider matrices of the form $\mathbf{K}_x + \alpha \mathbf{M}_x$, which are required to be positive definite. Therefore, the positivity of α can be relaxed in the case that $|\Gamma_D| > 0$.

Remark 3.2. A more detailed investigation of (3.4) shows that

$$\alpha = 0 \Longleftrightarrow x(0) = x(T) = y(0) = y(T) = 0, \tag{3.8}$$

for the eigenvector $\mathbf{z} = \mathbf{x} + \imath\mathbf{y}$ corresponding to $\alpha + \imath\beta$.

For the case $p = 1$, one can even show that for an eigenvector corresponding to an purely imaginary eigenvalue the property $x(0) = x(T) = y(0) = y(T) = 0$ cannot hold. Considering a uniform knot vector in $[0, 1]$ with B-Splines of degree $p = 1$ and $N_t \geq 3$, it holds

$$\mathbf{K}_t = \frac{1}{2}\begin{bmatrix} 1 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -1 & 0 & 1 & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{M}_t = C_n \begin{bmatrix} 2 & 1 & & & & \\ 1 & 4 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & 4 & 1 & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 2 \end{bmatrix},$$

where $C_n > 0$ depends on N_t. Rewriting $\mathbf{K}_t\mathbf{z} = \imath\beta\mathbf{M}_t\mathbf{z}$ as recurrence relation for $\mathbf{z} = [z_1, z_2, \ldots, z_{N_t-1}, z_{N_t}]$, we obtain

$$\begin{aligned} z_1 + z_2 &= \imath\beta(2z_1 + z_2) \\ -z_{i-1} + z_{i+1} &= \imath\beta(z_{i-1} + 4z_i + z_{i+1}) \quad i = 2, \ldots, N_t - 1 \\ -z_{N_t-1} + z_{N_t} &= \imath\beta(z_{N_t-1} + 2z_{N_t}), \end{aligned} \tag{3.9}$$

where we put the real number C_n and the $1/2$ in front of $\mathbf{K}_t$ into the eigenvalue $\imath\beta$. In order for $\mathbf{z} = [0, z_2, \ldots, z_{N_t-1}, 0]$ to be an eigenvector, we obtain from the first line of (3.9)

$$z_2 = \imath\beta z_2 \Leftrightarrow (1 - \imath\beta)z_2 = 0.$$

Since $(1-\imath\beta)$ cannot be zero, the only possibility for this equation to hold is when $z_2 = 0$. Considering now the second line of (3.9) and assuming $z_1 = \ldots = z_j = 0$, then, for $i = j$, the equation reads

$$z_{j+1} = \imath\beta z_{j+1} \Leftrightarrow (1 - \imath\beta)z_{j+1} = 0.$$

Therefore, $z_{j+1} = 0$. By induction it follows that $z = 0$. Hence, it cannot be an eigenvector.

In the case of $p > 1$, the matrices $\mathbf{K}_t$ and $\mathbf{M}_t$ have more than one off diagonal and such a relation would not follow so easily. Numerical experiments in Section 4.2 indicate that the real part of λ is positive for the case $p > 1$ too.

Remark 3.3. Let us consider the case $|\Gamma_D| > 0$. From Remark 3.1, Proposition 3.1 and the continuous dependence of α on θ, we obtain that $\mathbf{K}_x + \alpha\mathbf{M}_x$ must be positive for sufficiently small θ.

Remark 3.4. Numerical experiments for various values of θ, p and h_n in Section 4.2 indicate that the generalized eigenvalues λ_i have a positive real part α provided that the real part of the eigenvalues of $\mathbf{M}_t$ is positive. Moreover, in the practical implementation, one has to compute the eigenvalues λ_i anyway. Therefore, we always have an a posteriori control on the positivity of α. If it happens that $\alpha \leq 0$, than we have to use a smaller θ.

3.3 Diagonalization

If the matrix $\mathbf{M}_t^{-1}\mathbf{K}_t$ is diagonalizable, the eigenvalue decomposition allows us to write

$$\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{X}^{-1}\mathbf{D}\mathbf{X}, \tag{3.10}$$

where $\mathbf{D} = \mathrm{diag}(\lambda_i)$, $\lambda_i \in \mathbb{C}$, is a diagonal matrix with possibly complex eigenvalues on the diagonal, and $\mathbf{X} \in \mathbb{C}^{N_t \times N_t}$ denotes the matrix of the possibly complex eigenvectors. Due to the fact that the matrix $\mathbf{M}_t^{-1}\mathbf{K}_t$ is non-symmetric, the eigenvectors do not form an orthogonal basis, i.e. $X^{-1} \neq X^H$. An efficient calculation can be performed by means of solving the generalized eigenvalue problem $\mathbf{K}_t x = \lambda\mathbf{M}_t x$.

Thanks to (3.10), the matrix $(\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1}$ from (3.1) takes the form

$$(\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} = (\mathbf{D} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} = \mathrm{diag}_{i=1,\ldots,N_t}((\mathbf{K}_x + \lambda_i\mathbf{M}_x)^{-1}).$$

Therefore, only N_t problems of the form $(\mathbf{K}_x + \lambda_i \mathbf{M}_x)$ have to be solved, independently of each other. We have to distinguish two cases: the first case where the eigenvalue λ_i is a positive real number, and the second one where λ_i is a complex number.

In the first case, we consider $\lambda_i = \alpha_i \in \mathbb{R}^+$. In this case the matrix $\mathbf{K}_x + \lambda_i \mathbf{M}_x$ is symmetric positive definite. This allows for many possible exact and inexact solution strategies, e.g., Multigrid, Domain Decomposition type methods.

The second case, where $\lambda_i = \alpha + \imath\beta \in \mathbb{C}$ with $\alpha, \beta \in \mathbb{R}, \alpha > 0$, is more difficult to handle. We note that $(\mathbf{K}_x + \lambda_i \mathbf{M}_x)^H \neq \mathbf{K}_x + \lambda_i \mathbf{M}_x$. Separating the real and imaginary parts, we can rewrite the complex system $(\mathbf{K}_x + \lambda_i \mathbf{M}_x)z = h$ as a real system with a real block system matrix of twice size.

$$
\begin{aligned}
& (\mathbf{K}_x + \lambda_i \mathbf{M}_x)z = h \\
\iff & \begin{bmatrix} \mathbf{K}_x + \alpha_i \mathbf{M}_x & -\beta \mathbf{M}_x \\ \beta \mathbf{M}_x & \mathbf{K}_x + \alpha_i \mathbf{M}_x \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \\
\iff & \underbrace{\begin{bmatrix} \mathbf{K}_x + \alpha_i \mathbf{M}_x & \beta_i \mathbf{M}_x \\ \beta_i \mathbf{M}_x & -(\mathbf{K}_x + \alpha_i \mathbf{M}_x) \end{bmatrix}}_{=:\overline{A}_i} \begin{bmatrix} x \\ -y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix},
\end{aligned}
$$

where $z = x + \imath y$ and $h = f + \imath g$. The matrix $\overline{A}_i \in \mathbb{R}^{2N_x \times 2N_x}$ is symmetric, but indefinite. We are now looking for an robust preconditioner for $\overline{A}_i$. In order to construct such a preconditioner, we use operator interpolation technique, see, e.g., [33], [4] and [1]. First, we need the definition of the geometric mean of two operators and the general operator interpolation theorem, see also Definition. 2.28 and Theorem. 2.29 in [32].

Definition 1. *Let A and B be real, symmetric and positive definite matrices. We define the geometric mean of A and B by the relation*

$$[A, B]_{1/2} = A^{1/2}\big(A^{-1/2} B A^{-1/2}\big)^{1/2} A^{1/2}.$$

Moreover, for any $\vartheta \in [0, 1]$, we define the symmetric and positive matrix by

$$[A, B]_{\vartheta} = A^{1/2}\big(A^{-1/2} B A^{-1/2}\big)^{\vartheta} A^{1/2}.$$

Theorem 3.1. *Let $\mathcal{A} : \mathbb{R}^n \to \mathbb{R}^n$ such that the inequalities*

$$\underline{c}_0 \|u\|_{X_0} \leq \|\mathcal{A}u\|_{Y_0} \leq \overline{c}_0 \|u\|_{X_0} \quad \text{and} \quad \underline{c}_1 \|u\|_{X_1} \leq \|\mathcal{A}u\|_{Y_1} \leq \overline{c}_1 \|u\|_{X_1} \quad \forall u \in \mathbb{R}^n$$

hold, where the linear vector spaces $X_j = \mathbb{R}^n$ and $Y_j = \mathbb{R}^n$ with $j \in \{0, 1\}$ are equipped with the norms $\|\cdot\|_{X_j}$ and $\|\cdot\|_{Y_j}$, which are associated to the inner products

$$(u, v)_{X_j} = (M_j u, v)_{\ell_2} \quad \text{and} \quad (u, v)_{Y_j} = (N_j u, v)_{\ell_2},$$

given by the symmetric and positive definite matrices M_0, M_1, N_0 and N_1, and the euclidean inner product $(\cdot, \cdot)_{\ell_2}$. Then, for $X_\vartheta = [X_0, X_1]_\vartheta$ and $Y_\vartheta = [Y_0, Y_1]_\vartheta$, with $\vartheta \in [0, 1]$, the inequalities

$$\underline{c}_0^{1-\vartheta} \underline{c}_1^{\vartheta} \|u\|_{X_\vartheta} \leq \|\mathcal{A}u\|_{Y_\vartheta} \leq \overline{c}_0^{1-\vartheta} \overline{c}_1^{\vartheta} \|u\|_{X_\vartheta} \quad \forall u \in \mathbb{R}^n. \tag{3.11}$$

hold, where the norms $\|\cdot\|_{X_\vartheta}$ and $\|\cdot\|_{Y_\vartheta}$ are the norms associated to the inner products

$$
\begin{aligned}
(u, v)_{X_\vartheta} &= (M_\vartheta u, v)_{\ell_2}, \quad \text{with} \quad M_\vartheta = [M_0, M_1]_\vartheta, \quad \text{and} \\
(u, v)_{Y_\vartheta} &= (N_\vartheta u, v)_{\ell_2}, \quad \text{with} \quad N_\vartheta = [N_0, N_1]_\vartheta,
\end{aligned}
$$

respectively.

Proof. For the proof, we refer to the proof of Theorem 2.29 in [32] and references therein, see also [1]. □

Remark 3.5. Using the notation from Theorem 3.1, one can show the alternative representation

$$\|u\|_{X_\vartheta}^2 = \frac{2\sin(\vartheta\pi)}{\pi}\int_0^\pi t^{-(2\vartheta+1)}K(t;u)^2\,dt$$

of $\|u\|_{X_\vartheta}$, where $K(t;x) = \inf_{x=x_0+x_1}(\|x_0\|_{X_0}^2 + t^2\|x_1\|_{X_1}^2)^{1/2}$. From this representation, one observes that

$$[X_0, X_1]_\vartheta = [X_1, X_0]_{1-\vartheta}. \tag{3.12}$$

Let us consider a general saddle point matrix

$$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & -C \end{bmatrix},$$

where A and C are symmetric positive definite matrices. We can define two possible negative Schur complements

$$S := C + BA^{-1}B^T \quad \text{and} \quad R := A + BC^{-1}B, \tag{3.13}$$

and the associated block diagonal preconditioners

$$P_0 = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \quad \text{and} \quad P_1 = \begin{bmatrix} R & 0 \\ 0 & C \end{bmatrix}.$$

For P_0 and P_1, the following spectral inequalities are known

$$(\sqrt{5}-1)/2\|u\|_{P_j} \le \|\mathcal{A}u\|_{P_j^{-1}} \le (\sqrt{5}+1)/2\|u\|_{P_j} \quad j \in \{0,1\},$$

see Theorem 2.26 in [32] and references therein. Based on these two preconditioners, we construct a preconditioner P_ϑ with $\vartheta = 1/2$ by an interpolation of the preconditioners P_0 and P_1:

$$P_{1/2} = [P_0, P_1]_{1/2} = \begin{bmatrix} [A,R]_{1/2} & 0 \\ 0 & [S,C]_{1/2} \end{bmatrix}.$$

By means of Theorem 3.1 and the setting $M_0 = P_0, M_1 = P_1, N_0 = P_0^{-1}$ and $N_1 = P^{-1}$, it follows that

$$(\sqrt{5}-1)/2\|u\|_{P_{1/2}} \le \|\overline{A}u\|_{P_{1/2}^{-1}} \le (\sqrt{5}+1)/2\|u\|_{P_{1/2}}.$$

Hence, $\mathrm{cond}_{P_{1/2}}(P_{1/2}^{-1}\mathcal{A}) \le (\sqrt{5}+1)/(\sqrt{5}-1)$. Note, this condition number estimate would hold for all $\vartheta \in [0,1]$. In the following, we are looking for an approximation of $P_{1/2}$, which can easily be realized in an implementation.

Theorem 3.2. *Let K_x and M_x be symmetric and positive matrices, and let α and β be real numbers with $\alpha > 0$. Furthermore, we define the block matrices*

$$\overline{A} := \begin{bmatrix} \mathbf{K}_x + \alpha\mathbf{M}_x & \beta\mathbf{M}_x \\ \beta\mathbf{M}_x & -(\mathbf{K}_x + \alpha\mathbf{M}_x) \end{bmatrix}, \tag{3.14}$$

$$P := \begin{bmatrix} \mathbf{K}_x + (\alpha + |\beta|)\mathbf{M}_x & 0 \\ 0 & \mathbf{K}_x + (\alpha + |\beta|)\mathbf{M}_x \end{bmatrix}. \tag{3.15}$$

Then the condition number estimate

$$cond_P(P^{-1}\overline{A}) \leq \sqrt{2}\frac{\sqrt{5}+1}{\sqrt{5}-1} \tag{3.16}$$

holds.

Proof. The proof follows the lines in [32], Section 3.3. For simplicity, we introduce the notations $\mathcal{K} := \mathbf{K}_x + \alpha\mathbf{M}_x$ and $\mathcal{M} := \mathbf{M}_x$. Recall the system matrix

$$\overline{A} := \begin{bmatrix} \mathbf{K}_x + \alpha\mathbf{M}_x & \beta\mathbf{M}_x \\ \beta\mathbf{M}_x & -(\mathbf{K}_x + \alpha\mathbf{M}_x) \end{bmatrix} = \begin{bmatrix} \mathcal{K} & \beta\mathcal{M} \\ \beta\mathcal{M} & -\mathcal{K} \end{bmatrix}.$$

Since $\mathcal{K}$ is symmetric and, due to $\alpha > 0$, also positive definite, we can reformulate the two Schur complements from (3.13) for the matrix $\overline{A}$ as follows:

$$S = R = \mathcal{K} + \beta^2\mathcal{M}\mathcal{K}^{-1}\mathcal{M}.$$

We are looking for an spectral equivalent approximation P of $P_{1/2}$, which is easy to realize and fulfils the spectral inequalities

$$\underline{c}P \leq P_{1/2} \leq \overline{c}P, \tag{3.17}$$

where the constants $\underline{c}$ and $\overline{c}$ are independent of α and β. Next we estimate $[\mathcal{K}, R]_{1/2}$ and $[S, \mathcal{K}]_{1/2}$. Here we make use of the following matrix inequalities

$$\frac{1}{\sqrt{2}}(\sqrt{a}I + \sqrt{b}X^{1/2}) \leq (aI + bX)^{1/2} \leq \sqrt{a}I + \sqrt{b}X^{1/2}, \tag{3.18}$$

where X is a symmetric positive definite matrix, and I denotes the identity matrix. First we derive an upper bound for $[\mathcal{K}, R]_{1/2}$:

$$\begin{aligned}
[\mathcal{K}, R]_{1/2} &= \mathcal{K}^{1/2}\big(\mathcal{K}^{-1/2}R\mathcal{K}^{-1/2}\big)^{1/2}\mathcal{K}^{1/2} \\
&= \mathcal{K}^{1/2}\big(\mathcal{K}^{-1/2}(\mathcal{K} + \beta^2\mathcal{M}\mathcal{K}^{-1}\mathcal{M})\mathcal{K}^{-1/2}\big)^{1/2}\mathcal{K}^{1/2} \\
&= \mathcal{K}^{1/2}\big(I + \beta^2\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2}\big)^{1/2}\mathcal{K}^{1/2} \\
&\leq \mathcal{K}^{1/2}\big(I + (\beta^2\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2})^{1/2}\big)\mathcal{K}^{1/2} \\
&= \mathcal{K} + |\beta|\mathcal{K}^{1/2}(\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2})^{1/2}\mathcal{K}^{1/2} \\
&= \mathcal{K} + |\beta|\mathcal{K}^{1/2}(\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1/2})^{1/2}(\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1/2})^{1/2}\mathcal{K}^{1/2} \\
&= \mathcal{K} + |\beta|\mathcal{K}^{1/2}(\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1/2})\mathcal{K}^{1/2} \\
&= \mathcal{K} + |\beta|\mathcal{M}.
\end{aligned}$$

Similarly, for the lower bound, we obtain

$$\begin{aligned}
[\mathcal{K}, R]_{1/2} &= \mathcal{K}^{1/2}\big(\mathcal{K}^{-1/2} R \mathcal{K}^{-1/2}\big)^{1/2}\mathcal{K}^{1/2} \\
&= \mathcal{K}^{1/2}\big(I + \beta^2 \mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2}\big)^{1/2}\mathcal{K}^{1/2} \\
&\geq \mathcal{K}^{1/2}\big(\frac{1}{\sqrt{2}}(I + (\beta^2 \mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2})^{1/2})\big)\mathcal{K}^{1/2} \\
&= \frac{1}{\sqrt{2}}(\mathcal{K} + |\beta|\mathcal{K}^{1/2}(\mathcal{K}^{-1/2}\mathcal{M}\mathcal{K}^{-1}\mathcal{M}\mathcal{K}^{-1/2})^{1/2}\mathcal{K}^{1/2}) \\
&= \frac{1}{\sqrt{2}}(\mathcal{K} + |\beta|\mathcal{M}).
\end{aligned}$$

The missing estimate from above and below for $[S, \mathcal{K}]_{1/2}$ follow from the fact that $[S, \mathcal{K}]_{1/2} = [\mathcal{K}, S]_{1/2} = [\mathcal{K}, R]_{1/2}$, see (3.12). Hence, for the preconditioner

$$P := \begin{bmatrix} \mathcal{K} + |\beta|\mathcal{M} & 0 \\ 0 & \mathcal{K} + |\beta|\mathcal{M} \end{bmatrix} = \begin{bmatrix} \mathbf{K}_x + (\alpha + |\beta|)\mathbf{M}_x & 0 \\ 0 & \mathbf{K}_x + (\alpha + |\beta|)\mathbf{M}_x \end{bmatrix},$$

we obtain the spectral constants $\underline{c} = \frac{1}{\sqrt{2}}$ and $\overline{c} = 1$ in (3.17). Finally, we arrive at the estimate

$$\mathrm{cond}_P(P^{-1}\overline{A}) = \|P^{-1}\overline{A}\|_P \|\overline{A}^{-1}P\|_P \leq \sqrt{2}\|P_{1/2}^{-1}\overline{A}\|_{P_{1/2}}\|\overline{A}^{-1}P_{1/2}\|_{P_{1/2}} \leq \sqrt{2}\frac{\sqrt{5}+1}{\sqrt{5}-1}. \tag{3.19}$$

□

Remark 3.6. The estimate (3.19) of the condition number $\mathrm{cond}_P(P^{-1}\overline{A})$ can be improved by solving the generalized eigenvalue problem

$$\overline{A}\begin{bmatrix} x \\ y \end{bmatrix} = \lambda P \begin{bmatrix} x \\ y \end{bmatrix}$$

directly. Following the procedure outlined in Remark 9 in [33], see also the proof of Theorem 3.3, we find that the generalized eigenvalues satisfy the estimates

$$|\lambda_{min}| \geq \frac{1}{\sqrt{2}} \quad \text{and} \quad |\lambda_{max}| \leq 1,$$

which leads to the condition number estimate $\mathrm{cond}_P(P^{-1}A) \leq \sqrt{2}$.

We note that both block-diagonal entries of P are identical, and the matrix $\mathbf{K}_x + (\alpha + |\beta|)\mathbf{M}_x$ is symmetric and positive definite. This opens various possibilities for preconditioning based on standard techniques for symmetric and positive definite matrices. The linear system $\overline{A}y = f$ can then be solved, e.g., by means of MinRes preconditioned by P^{-1}. We can even use an spectral equivalent approximation $\hat{P}^{-1}$, i.e., $c\hat{P}^{-1} \leq P^{-1} \leq C\hat{P}^{-1}$, with constants c and C, independent of α and β. Moreover, this approach allows for a further parallelization by applying $\mathbf{A}_n$ in parallel for $n = 1, \ldots, N_t$.

Unfortunately, this approach has a severe drawback. Due to the fact that the matrix $\mathbf{M}_t^{-1}\mathbf{K}_t$ is non-symmetric, the matrix $\mathbf{X}$ of eigenvectors is not unitary and, therefore, $\mathrm{cond}(\mathbf{X}) \neq 1$. Actually, numerical tests in Section 4.1 show that, for large B-Spline degree or small h_t, we observe that the condition number $\mathrm{cond}(\mathbf{X}) \approx 10^{12}$. In that case we cannot correctly apply (3.1) and the algorithm fails. This problem can be circumvented by using the Complex or Real Schur decomposition, as presented in the subsequent two subsections.

3.4 Complex Schur decomposition

In this section, we investigate an alternative possibility for decomposing $\mathbf{M}_t^{-1}\mathbf{K}_t$. The Complex Schur decomposition provides a decomposition of the form

$$\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{Q}^*\mathbf{T}\mathbf{Q}, \tag{3.20}$$

where $\mathbf{Q} \in \mathbb{C}^{N_t \times N_t}$ and $\mathbf{T} \in \mathbb{C}^{N_t \times N_t}$ is a upper triangular matrix with $T_{ii} = \lambda_i$. The advantage of the (complex) Schur decomposition is the fact that we obtain a unitary matrix $\mathbf{Q}$. Hence, $\text{cond}(\mathbf{Q}) = 1$, but the diagonal matrix $\mathbf{D}$ in the decomposition (3.10) is now replaced by the upper triangular matrix $\mathbf{T}$ in the decomposition (3.20), By means of (3.20), the matrix $\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x$ from (3.1) takes the form

$$\begin{aligned}
(\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} &= (\mathbf{T} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} \\
&= \begin{bmatrix} \mathbf{K}_x + T_{11}\mathbf{M}_x & T_{12}\mathbf{M}_x & \dots & \\ 0 & \mathbf{K}_x + T_{22}\mathbf{M}_x & T_{23}\mathbf{M}_x & \\ \vdots & 0 & \ddots & T_{N_tN_t-1}\mathbf{M}_x \\ 0 & \dots & 0 & \mathbf{K}_x + T_{N_tN_t}\mathbf{M}_x \end{bmatrix}^{-1} \\
&= \begin{bmatrix} \mathbf{K}_x + \lambda_1\mathbf{M}_x & T_{12}\mathbf{M}_x & \dots & \\ 0 & \mathbf{K}_x + \lambda_2\mathbf{M}_x & T_{23}\mathbf{M}_x & \\ \vdots & 0 & \ddots & T_{N_tN_t-1}\mathbf{M}_x \\ 0 & \dots & 0 & \mathbf{K}_x + \lambda_{N_t}\mathbf{M}_x \end{bmatrix}^{-1}
\end{aligned}$$

The application of $(\mathbf{T} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1}$ to some vector f can be performed staggered way as presented in Algorithm 1.

Algorithm 1 Calculation of $y = (\mathbf{T} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} f$

```
for i = N_t, N_t − 1 ..., 1 do
    g = f_i
    for j = i + 1, i + 2 ..., N_t do
        g = g − T_ij y_j
    end for
    Solve (K_x + λ_i M_x) y_i = g, where λ_i = T_ii.
end for
return y
```

In order to solve the linear systems $(\mathbf{K}_x + \lambda_i\mathbf{M}_x)y_i = g, i = 1, \dots, N_t$ in Algorithm 1, we can use the techniques developed in the previous subsection. This decomposition method allows us to have a well conditioned transformation matrix Q, however at the cost that the linear system cannot be solved independently of each other. We note that this method and the eigenvalue decomposition require complex arithmetic, which is more expensive than the real one. In the following subsection, we investigate the real Schur decomposition, which eliminates the need for having complex arithmetic.

3.5 Real Schur decomposition

In this subsection, we look at the decomposition of $\mathbf{M}_t^{-1}\mathbf{K}_t$ by means of the Real Schur decomposition. It provides a decomposition of the form

$$\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{Q}^*\mathbf{T}\mathbf{Q}, \tag{3.21}$$

where $\mathbf{Q} \in \mathbb{R}^{N_t \times N_t}$. The matrix $\mathbf{T} \in \mathbb{R}^{N_t \times N_t}$ is a upper quasi-triangular matrix, i.e., the diagonal consists of 1×1 and 2×2 blocks. The values of the 1×1 blocks correspond to the real eigenvalues, while the 2×2 blocks correspond to the complex eigenvalues of $\mathbf{M}_t^{-1}\mathbf{K}_t$.

By additionally performing a Givens rotation, the 2×2 block can be transformed to the structure

$$\mathbf{B} := \begin{bmatrix} \alpha & \beta_1 \\ \beta_2 & \alpha \end{bmatrix},$$

where $\alpha, \beta_1, \beta_2 \in \mathbb{R}$ and $\beta_1 \neq \beta_2 \neq 0$. The eigenvalues of this matrix are given by $\alpha \pm \sqrt{\beta_1\beta_2}$. Due to the fact that the eigenvalues have to be complex and the real part has to be positive, we obtain that $\alpha > 0$ and β_1 and β_2 have different signs. Therefore, we can write the eigenvalues as $\alpha \pm \imath\sqrt{|\beta_1\beta_2|}$.

Using this decomposition, the matrix $\mathbf{Z} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x$ appearing in (3.1) has a structure, which is similar to that one of the Complex Schur decomposition. The corresponding system of linear algebraic equations can also be again solved in a staggered way as presented in Algorithm 1. One has to adapt the algorithm in such a way that, if the diagonal block is a 2×2 block, one has to work with two-block vectors and a 2×2 block matrix. It remains to investigate the solution strategy for the 2×2 block matrix. As already mentioned, the 2×2 block of T is non-symmetric. Hence, the 2×2 block matrix is also non-symmetric and is given in the following way

$$\begin{bmatrix} \mathbf{K}_x + \alpha\mathbf{M}_x & \beta_1\mathbf{M}_x \\ \beta_2\mathbf{M}_x & \mathbf{K}_x + \alpha\mathbf{M}_x \end{bmatrix}.$$

The structure of the matrix is very similar to $\overline{A}$ in Theorem 3.2 up to the non-symmetry, which origins just from the different scalings β_1 and β_2 and their different sign. By a proper rescaling, we can transform this linear system into an equivalent system with a symmetric, but indefinite system matrix:

$$\begin{aligned} \begin{bmatrix} \mathbf{K}_x + \alpha\mathbf{M}_x & \beta_1\mathbf{M}_x \\ \beta_2\mathbf{M}_x & \mathbf{K}_x + \alpha\mathbf{M}_x \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &= \begin{bmatrix} f \\ g \end{bmatrix} \\ \iff \begin{bmatrix} \mathbf{K}_x + \alpha\mathbf{M}_x & -\beta_1\mathbf{M}_x \\ \beta_2\mathbf{M}_x & -(\mathbf{K}_x + \alpha\mathbf{M}_x) \end{bmatrix} \begin{bmatrix} x \\ -y \end{bmatrix} &= \begin{bmatrix} f \\ g \end{bmatrix} \\ \iff \underbrace{\begin{bmatrix} |\beta_2|(\mathbf{K}_x + \alpha\mathbf{M}_x) & -\beta_1|\beta_2|\mathbf{M}_x \\ |\beta_1|\beta_2\mathbf{M}_x & -|\beta_1|(\mathbf{K}_x + \alpha\mathbf{M}_x) \end{bmatrix}}_{=:\overline{A}} \begin{bmatrix} x \\ -y \end{bmatrix} &= \begin{bmatrix} |\beta_2|f \\ |\beta_1|g \end{bmatrix}, \end{aligned}$$

We note that β_1 and β_2 have different signs. Hence, $-\beta_1|\beta_2| = -\beta_2|\beta_1|$. Motivated by the construction of the preconditioner in the case of the eigenvalue decomposition, we can come up with an optimal preconditioner. The following theorem presents this optimal preconditioner for the matrix $\overline{A}$.

Theorem 3.3. *Let K_x and M_x be symmetric and positive matrices, and let α, β_1, β_2 be real numbers with $\alpha > 0$. Furthermore, we define the block matrices*

$$\begin{aligned} \overline{A} &:= \begin{bmatrix} |\beta_2|(\mathbf{K}_x + \alpha\mathbf{M}_x) & -\beta_1|\beta_2|\mathbf{M}_x \\ |\beta_1|\beta_2\mathbf{M}_x & -|\beta_1|(\mathbf{K}_x + \alpha\mathbf{M}_x) \end{bmatrix}, \\ P &:= \begin{bmatrix} |\beta_2|(\mathbf{K}_x + (\alpha + \sqrt{|\beta_1\beta_2|})\mathbf{M}_x) & 0 \\ 0 & |\beta_1|(\mathbf{K}_x + (\alpha + \sqrt{|\beta_1\beta_2|})\mathbf{M}_x) \end{bmatrix}. \end{aligned}$$

Then the condition number estimate

$$cond(P^{-1}\overline{A}) \leq \sqrt{2}.$$

holds.

Proof. The proof follows the lines from Remark 9 in [33], which gives a sharper bound than using interpolation theory as in [32]. For notational simplicity, we introduce the abbreviations $\mathcal{K} := \mathbf{K}_x + \alpha\mathbf{M}_x$ and $\mathcal{M} := \mathbf{M}_x$. We now consider the generalized eigenvalue problem $\overline{A}u = \lambda Pu$, which reads

$$\begin{bmatrix} |\beta_2|\mathcal{K} & -\beta_1|\beta_2|\mathcal{M} \\ |\beta_1|\beta_2\mathcal{M} & -|\beta_1|\mathcal{K} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} |\beta_2|(\mathcal{K} + \sqrt{|\beta_1\beta_2|}\mathcal{M}) & 0 \\ 0 & |\beta_1|(\mathcal{K} + \sqrt{|\beta_1\beta_2|}\mathcal{M}) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}. \tag{3.22}$$

At first we consider the generalized eigenvalue problem

$$\mathcal{K}z = \mu(\mathcal{K} + \sqrt{|\beta_1\beta_2|}\mathcal{M})z.$$

Due to the fact that $\mathcal{K}$ and $\mathcal{M}$ are symmetric, there exists an basis $\{e_1, e_2, \ldots, e_{N_x}\}$ of eigenvectors, which are orthonormal with respect to the inner product generated by $\mathcal{K}+\sqrt{|\beta_1\beta_2|}\mathcal{M}$, and corresponding eigenvalues μ_j. Since $\mathcal{K}$ is dominated by $\mathcal{K}+\sqrt{|\beta_1\beta_2|}\mathcal{M}$ and due to their positivity, we have that $\mu_j \in [0, 1]$. Therefore, we can express x and y as linear combination of e_j with coefficients $\hat{x}_j$ and $\hat{y}_j$, respectively. Moreover, $\mathcal{M}z$ fulfils the following identity

$$\begin{aligned} \mathcal{M}z &= (|\beta_1\beta_2|)^{-1/2}(\sqrt{|\beta_1\beta_2|}\mathcal{M} + \mathcal{K})z - (|\beta_1\beta_2|)^{-1/2}\mathcal{K}z \\ &= (|\beta_1\beta_2|)^{-1/2}(\sqrt{|\beta_1\beta_2|}\mathcal{M} + \mathcal{K})z - (|\beta_1\beta_2|)^{-1/2}\mu(\mathcal{K} + \sqrt{|\beta_1\beta_2|}\mathcal{M})z \\ &= (|\beta_1\beta_2|)^{-1/2}(1-\mu)(\sqrt{|\beta_1\beta_2|}\mathcal{M} + \mathcal{K})z. \end{aligned}$$

Using the expansion of x and y into the eigenvectors $\{e_j\}$, system (3.22) decomposes into the 2×2 systems

$$\begin{bmatrix} |\beta_2|\mu_j & -\beta_1|\beta_2||\beta_1\beta_2|^{-1/2}(1-\mu_j) \\ |\beta_1|\beta_2|\beta_1\beta_2|^{-1/2}(1-\mu_j) & -|\beta_1|\mu_j \end{bmatrix} \begin{bmatrix} \hat{x}_j \\ \hat{y}_j \end{bmatrix} = \lambda \begin{bmatrix} |\beta_2| & 0 \\ 0 & |\beta_1| \end{bmatrix} \begin{bmatrix} \hat{x}_j \\ \hat{y}_j \end{bmatrix}.$$

Since there exists at least one pair $(\hat{x}_j, \hat{y}_j)$ which is non-zero, the determinant of the system matrix must be zero, i.e.,

$$\det\left(\begin{bmatrix} |\beta_2|\mu_j & -\beta_1|\beta_2||\beta_1\beta_2|^{-1/2}(1-\mu_j) \\ |\beta_1|\beta_2|\beta_1\beta_2|^{-1/2}(1-\mu_j) & -|\beta_1|\mu_j \end{bmatrix} - \lambda \begin{bmatrix} |\beta_2| & 0 \\ 0 & |\beta_1| \end{bmatrix} \right) = 0,$$

which reduces to

$$|\beta_1\beta_2|(\lambda^2 - \mu_j^2) - (\beta_1\beta_2)^2|\beta_1\beta_2|^{-1}(1-\mu_j)^2 = 0,$$

where we used that $-\beta_1|\beta_2| = |\beta_1|\beta_2 \neq 0$. We immediately obtain that $|\lambda| = \sqrt{\mu_j^2 + (1-\mu_j)^2}$ for $\mu_i \in [0, 1]$ and it follows that $\frac{1}{\sqrt{2}} \leq |\lambda| \leq 1$, which gives the desired bound on the condition number of $P^{-1}\overline{A}$. □

Now we can again use the MinRes preconditioned by P as iterative solver for systems with the system matrix $\overline{A}$, and we obtain a robust method. Moreover, due to the use of real arithmetic, this approach is usually more efficient than that one using the Complex Schur decomposition.

4 Numerical examples

In this section, we test the proposed preconditioners on the three (2+1) dimensional space-time cylinder Q illustrated in Figure 1. The two dimensional spatial domain Ω consists of 21 spatial subdomains (volumetric patches). For each time slap, we use conforming B-Splines of degree p. The problems were calculated on a Desktop PC with an Intel(R) Xeon(R) CPU E5-1650 v2 @ 3.50GHz and 16 GB main memory. We use the C++ library G+Smo for describing the geometry and performing the numerical tests, see also [18] and [24].

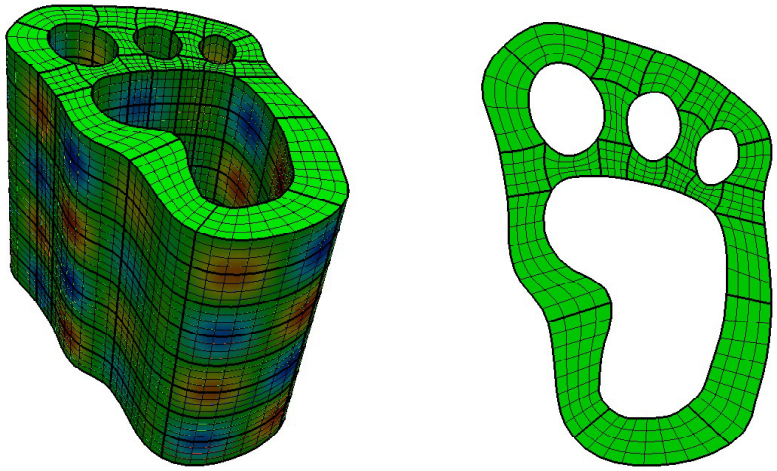

Fig. 1. The left picture shows the space-time cylinder Q with 8 time slabs, while the right picture presents the spatial domain Ω consisting of 21 patches.

4.1 Condition number of eigenvector matrix X

Here, we study the condition number of the generalized eigenvectors of $(\mathbf{K}_t, \mathbf{M}_t)$. Due to the non-symmetry of K_t and M_t, we do not obtain an orthogonal basis of eigenvectors. Hence, the condition number is not 1. Actually, it can be quite large. We report on the condition number for different p and N_t in Table 1. We observe that the condition number grows exponentially with p and N_t. We conclude that for small p or small number of dofs in time direction, the approach presented in Section 3.3 may be still feasible.

4.2 Smallest eigenvalue of $\mathbf{M}_t^{-1}\mathbf{K}_t$

In Section 3.2, we observed the necessity that the real part of the smallest eigenvalue of $\mathbf{M}_t^{-1}\mathbf{K}_t$ is positive. In this section, we present numerical studies for different p, h and θ, where we fix the time interval to $[0, 1]$. The results are summarized in Table 2, where the entries with $*$ indicate that the matrix M_t had at least one eigenvalue with negative real part. Consequently, the smallest real part of the generalized eigenvalues was also negative. We observe that, if $\mathbf{M}_t > 0$, then also the real part of $\mathbf{M}_t^{-1}\mathbf{K}_t$ is positive. The positive real part of the eigenvalues for the $p = 1$ and $\theta = 0$ is in agreement with Remark 3.2. Moreover, for $\theta = 0$ and increasing p we observe even an increase of the smallest real part

$N_t - p \setminus p$	2	3	4	5	6	7	8
2	64	309	362	766	1706	3907	9501
4	481	1036	3037	9419	41959	39323	73946
8	2869	16118	39693	74370	180054	472758	1e+06
16	34332	188263	463148	1e+06	6e+06	3e+07	1e+08
32	701306	2e+06	1e+07	6e+07	4e+08	7e+09	1e+10
64	5e+07	4e+07	3e+08	3e+09	6e+10	3e+11	1e+12
128	2e+08	1e+09	1e+10	3e+11	2e+13	5e+13	4e+14

Table 1. Condition number of $\mathbf{X}$ for $\theta = 0.01$ and $|t_{n+1} - t_n| = 0.1$.

of the eigenvalues, cf. Proposition 3.1 and Remark 3.2. The numerical tests indicate that, for sufficiently small θ, the smallest real part of the generalized eigenvalues stays positive.

	2 uniform refinements							4 uniform refinements						
$\theta \backslash p$	1	2	3	4	5	6	7	1	2	3	4	5	6	7
0	1.5	2.4	3.2	3.8	4.3	4.7	5.0	0.2	0.5	0.9	1.5	2.1	2.7	3.4
0.01	1.6	2.5	3.2	3.6	4.0	4.4	4.9	0.7	0.7	1.1	1.6	2.2	2.8	3.3
0.1	2.5	2.9	3.2	3.6	4.0	4.5	5.2	4.8	2.9	2.7	3.0	3.4	3.6	4.1
1	4.1	4.5	4.7	*	*	*	*	12.4	12.0	9.2	*	*	*	*
10	4.6	5.2	5.2	*	*	*	*	6.7	11.8	*	*	*	*	*
	6 uniform refinements							8 uniform refinements						
$\theta \backslash p$	1	2	3	4	5	6	7	1	2	3	4	5	6	7
0	0.01	0.03	0.06	0.1	0.1	0.2	0.2	0.0008	0.002	0.004	0.006	0.009	0.01	0.02
0.01	1.9	1.0	0.8	0.7	0.6	0.6	0.6	7.7	4.0	3.0	2.5	2.0	1.8	1.6
0.1	18.6	9.9	7.4	6.0	5.1	4.5	4.0	34.8	33.8	29.5	23.8	20.0	17.2	15.1
1	34.2	35.1	33.8	*	*	*	*	34.8	34.4	34.5	*	*	*	*
10	11.4	17.4	*	*	*	*	*	29.0	32.2	*	*	*	*	*

Table 2. Smallest real part of generalized eigenvalues $\mathbf{K}_t x = \lambda \mathbf{M}_t x$ for different B-Spline degrees p, θ and number of dofs. The $*$ indicates that the matrix $\mathbf{M}_t$ has at least one eigenvalue with negative real part.

4.3 Condition number of preconditioned $\mathbf{K}_x + \lambda \mathbf{M}_x$

The aim of this section is to verify the optimal condition number bound presented in Theorem 3.2 and Theorem 3.3. To do so, we report on the maximum number of MinRes-iterations in order to solve $\mathbf{K}_x + \lambda_i \mathbf{M}_x$, where $\lambda_i \in \mathbb{C}$ are the generalized eigenvalues of $(\mathbf{K}_t, \mathbf{M}_t)$. We use zero initial guess, and a reduction of the initial residual by 10^{-10}. We choose $\theta = 0.1$. In Table 3, we investigate the robustness of the preconditioners from Theorem 3.2 and Theorem 3.3. We observe that the number of iterations stays bounded for various p and h.

	Complex Schur decomp.					Real Schur decomp.				
ref. x and $t \setminus p$	2	3	4	5	6	2	3	4	5	6
0	23	22	26	26	26	18	18	20	21	22
1	25	24	24	27	26	20	20	22	22	22
2	25	25	25	27	27	22	22	22	22	22
3	24	26	26	27	27	22	22	22	22	21
4	25	25	26	27	26	22	22	22	22	20

Table 3. Maximum number of MinRes iterations to solve $\mathbf{K}_x+\lambda_i\mathbf{M}_x$, $i = 1, \ldots, N_t$, resulting from the Complex and Real Schur decomposition. Refinement is performed uniformly in x and t.

4.4 Application to Space-Time Multigrid

This section deals with the use of the iterative methods developed in Section 3.2 as smoothers in the space-time multigrid. The realization of the preconditioner P, see Theorem 3.2 and Theorem 3.3 is performed via a sparse direct solver. We use the PARDISO 5.0.0 Solver Project [19] for performing the LU factorizations. We compare the three different approaches, presented in Section 3.2, with the exact realization of $\mathbf{A}_n^{-1}$ via the sparse direct solver PARDISO. For approximating $\mathbf{A}_n^{-1}$ via MinRes, we use zero initial guess and a reduction of the initial residuum by 10^{-4}. In Table 4, we report on the single core computation time of the MG algorithm to setup the data-structures and solve the system via the MG iteration. The setup time includes the LU factorizations, but not the assembling of the matrices. For the MG iteration, we use zero initial guess and a reduction of the initial residuum by 10^{-8}. We choose $\theta = 0.01$, $|t_n - t_{n+1}| = 0.1$ and the polynomial degree by $p = 3$ for both space and time direction. Moreover, we fix the number of dofs in time direction of a time slab, but increase the number of time slabs. The MG method uses coarsening in space as well as in time.

We observe that the LU factorization of $\mathbf{A}_n$ needs a quite large amount of time, whereas the setup time is almost negligible for the three preconditioners proposed. The little increase in the solution time definitely pays off by the small setup time. In addition, the Real-Schur decomposition almost provides the same solution time as the direct solver. Due to the complex arithmetic of the Diagonalization or the Complex-Schur decomposition, their computational effort doubles, which we observe also in the numerical test. Finally, due to the quite accurate approximation of $\mathbf{A}_n^{-1}$ (up to 10^{-4}), we do not observe a deterioration of the MG iteration numbers. It took around 12 iterations to reach the desired tolerance of 10^{-4}.

5 Conclusions

In this work, we presented a decomposition of a non-symmetric linear system arising from a space-time formulation into a series of symmetric linear systems, which are easier to solve. These problems are part of the time-parallel MG method introduced in [25]. They correspond to spatial problems. They are either symmetric and positive definite or have a symmetric saddle point structure. For the latter, we presented robust preconditioners motivated by operator interpolation theory. The runtime performance is already very promising, even when using direct solvers, and can further be reduced by using robust

#dofs	ref		#slaps	MG-It	Direct		Diag	
	x	t			Setup	Solving	Setup	Solving
15950	2	3	2	7	1.9	0.7	0.04	2.3
97020	3	3	4	7	38.6	8.5	0.3	19.4
665720	4	3	8	7	1008	94.6	3.7	183.8
#dofs	ref		#slaps	MG-It	C-Schur		R-Schur	
15950	2	3	2	7	0.05	2.4	0.04	1.3
97020	3	3	4	7	0.5	19.9	0.3	11.1
665720	4	3	8	7	5.4	187.3	3.7	108.0

Table 4. Comparison of the Diagonalization as well as the Complex Schur and Real Schur decompositions with a sparse direct solver used for approximating $\mathbf{A}_n^{-1}$. All timings are given in seconds.

IgA multigrid or IgA domain decomposition approaches as proposed, e.g., in [10,11,12] or [14,15], respectively. The advantage of the decompositions proposed consists in the availability of well-established preconditioners for symmetric and positive definite problems.

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