Abstract

In this paper we propose a space-time least-squares isogeometric method to solve parabolic evolution problems, well suited for high-degree smooth splines in the space-time domain. We focus on the linear solver and its computational efficiency: thanks to the proposed formulation and to the tensor-product construction of space-time splines, we can design a preconditioner whose application requires the solution of a Sylvester-like equation, which is performed efficiently by the Fast Diagonalization method. The preconditioner is robust w.r.t. spline degree and meshsize. The computation time required for its application, for a serial execution, is almost proportional to the number of degrees-of-freedom and independent of the polynomial degree. The proposed approach is also well-suited for parallelization.

Keywords: Isogeometric analysis, parabolic problem, space-time method, k-method, splines, least-squares, Sylvester equation.

1 Introduction

Isogeometric Analysis (IGA) is a recent technique for the numerical solution of partial differential equations (PDE), introduced in the seminal paper [15]. IGA is an evolution of classical finite element methods (FEM): the main idea is to use the same functions (splines or generalizations) that represent the computational domain in Computer-Aided Design systems, also in the approximation of the solution. We refer to [7] and [4] for a comprehensive presentation and a mathematical survey of IGA, respectively.

IGA allows to use high-order and high-continuity functions. The \(k\)-method, based on splines of degree \(p\) and, typically, \(C^{p-1}\) regularity, delivers higher accuracy per degree-of-freedom, comparing to \(C^0\) or discontinuous \(hp\)-FEM. However, the \(k\)-method also requires ad-hoc algorithms, otherwise when the polynomial degree \(p\) increases, the computational cost per degree-of-freedom increases dramatically, both in the formation of the matrix and in the solution of the linear system.

In this paper we design and analyze an isogeometric method for parabolic equations, focusing on the heat equation as model problem.

Common numerical methods for time-dependent PDE are obtained by discretizing separately in time (e.g., by difference schemes) and in space (e.g., by a Galerkin method). We consider instead the alternative approach of discretizing the PDE simultaneously in space and time, that is, the so-called space-time (variational) approach. This approach has been pioneered in [16] in the context of finite elements, and later developed especially in the field of computational fluid dynamics, see for example the book [3]. The mathematical analysis of Galerkin space-time methods for parabolic equations has been developed in [27] for a wavelet discretization, and, more recently, in [29] for a Galerkin finite element discretization. In the IGA framework, the idea of using smooth splines in time has been first proposed in [31]. The recent paper [32] applies this concept to a complex engineering simulation. A stable space-time isogeometric method for the heat equation, based on the use of time-upwind test functions, has been proposed in [20, 21] and its time-parallel multigrid solver has been developed in [14].
The novelty of this paper is that we develop an isogeometric formulation that is suited for high degree and continuity splines in time and space, showing the potential of the k-method in space-time formulations. Our approach is based on a least-squares approximation of the PDE in space-time, which requires $C^1$-continuous functions in the spatial variable. The focus of this paper is the design of an efficient solver for the linear system that arises. Indeed, the reason for choosing a least-squares formulation is that it allows the use of the preconditioning technique introduced in [24] for the Poisson problem. Our preconditioner is based on the solution of a suitable Sylvester-like equation, by the so-called Fast Diagonalization (FD) method, originally proposed in [22] and more recently discussed in [9]. The computational cost of the preconditioner setup is at most $O(N_{dof})$ floating-point operations (FLOPs) while its application is $O(N_{dof}^{1+1/d})$ FLOPs, where $d$ is the number of space dimensions and $N_{dof}$ denotes the total number of degrees-of-freedom (for simplicity, here we consider the same number of degrees-of-freedom in time and in each space direction). In our numerical benchmarks, where we consider only serial single-core execution, the measured computation time of the preconditioner is close to optimality (about $O(N_{dof})$) and independent of $p$. Therefore, the preconditioner is robust with respect to the polynomial degree. In our simplest approach no information on the geometry parametrization is taken into account in the preconditioner setup: this results in a loss of efficiency with complicated domains. To overcome this issue, we also propose a more sophisticated preconditioner construction that partially incorporates some geometrical information, without increasing its computational complexity.

Space-time methods facilitate the full parallelization of the solver, see [12]. We do not address this important issue in our paper, but it will be the focus of our further research: indeed the preconditioner we propose fits in the framework, e.g., of [18].

The paper is organized as follows. In Section 2 we introduce B-Spline basis functions and the isogeometric spaces that we need for the discrete analysis. The parabolic model problem is presented in Section 3, where we also discuss the well-posedness of the least-squares approximation and the a-priori error estimates. Section 4 focuses on preconditioning strategies and their spectral analysis. We show numerical results to assess the performance of the proposed preconditioners and to confirm the a-priori error estimates in Section 6, while in the last section we draw some conclusions of our work and we highlight future research directions.

2 Preliminaries

2.1 B-splines

A knot vector in $[0, 1]$ is a sequence of non-decreasing points $\Xi := \{0 = \xi_1 \leq \cdots \leq \xi_{m+p+1} = 1\}$, where $m$ and $p$ are positive integers. We use open knot vectors, that is $\xi_1 = \cdots = \xi_{p+1} = 0$ and $\xi_m = \cdots = \xi_{m+p+1} = 1$. Then, according to Cox-De Boor recursion formulas (see [8]), the univariate B-splines are piecewise polynomials $b_{i,p}$ defined as

for $p = 0$:

$$\hat{b}_{i,0}(\eta) = \begin{cases} 1 & \text{if } \xi_i \leq \eta < \xi_{i+1}, \\ 0 & \text{otherwise}, \end{cases}$$

for $p \geq 1$:

$$\hat{b}_{i,p}(\eta) = \begin{cases} \frac{\eta - \xi_i}{\xi_{i+p} - \xi_i} \hat{b}_{i,p-1}(\eta) + \frac{\xi_{i+p+1} - \eta}{\xi_{i+p+1} - \xi_{i+1}} \hat{b}_{i+1,p-1}(\eta) & \text{if } \xi_i \leq \eta < \xi_{i+p+1}, \\ 0 & \text{otherwise}, \end{cases}$$

where we adopt the convention $0/0 = 0$. We define the univariate spline space as

$$\hat{S}_p^m := \text{span}\{\hat{b}_{i,p}\}_{i=1}^m$$

where $h$ denotes the meshsize. The smoothness of the B-splines at the knots depends on the knot multiplicity (for more details on B-splines and their use in isogeometric analysis, see [8] and [7]).

Multivariate B-splines are defined as tensor product of univariate B-splines. We will consider functions of space and time, where the space domain is $d$-dimensional. Therefore we introduce $d+1$ univariate knot
vectors $\Xi_l := \{\xi_{l,1}, \ldots, \xi_{l,m_l+p_l+1}\}$ for $l = 1, \ldots, d$ and $\Xi := \{\xi_{1,1}, \ldots, \xi_{m+1}\}$. We collect the degree indexes in a vector $p := (p_s, p_t)$, where $p_s := (p_1, \ldots, p_d)$ and for simplicity, we suppose $p_1 = \cdots = p_d = p_s$.

In the following, $h_s$ will denote the maximum meshsize in all spatial direction and $h_t$ the meshsize in the time direction. We assume that a quasi-uniformity condition on the knot vectors holds.

**Assumption 1.** We assume that the knot vectors are quasi-uniform, that is, there exists $\alpha > 0$, independent of $h_s$ and $h_t$, such that each non-empty knot span $(\xi_{l,i}, \xi_{l,i+1})$ fulfills $\alpha h_s \leq \xi_{l,i+1} - \xi_{l,i} \leq h_s$, for $1 \leq l \leq d$, and each non-empty knot span $(\xi_{t,i}, \xi_{t,i+1})$ fulfills $\alpha h_t \leq \xi_{t,i+1} - \xi_{t,i} \leq h_t$.

We denote by $\hat{\Omega} := [0,1]^d$ the spatial parameter domain. We define the multivariate B-splines on $\hat{\Omega} \times [0,1]$ as

$$\hat{B}_{i,p}(\eta, \tau) := \hat{B}_{i,s,h}(\eta) \hat{B}_{i,t,h}(\tau),$$

where $\hat{B}_{i,s,h}(\eta) := \hat{b}_{i_1,p_1}(\eta_1) \cdots \hat{b}_{i_d,p_d}(\eta_d)$, $i := (i_1, \ldots, i_d)$, $i := (i_s, i_t)$ and $\eta := (\eta_1, \ldots, \eta_d)$. The corresponding spline space is defined as

$$\hat{S}^p_h := \left\{ \hat{B}_{i,p} \mid i_k = 1, \ldots, m_k \text{ for } k = 1, \ldots, d; i_t = 1, \ldots, m_t \right\},$$

where $\hat{h} := \max\{h_s, h_t\}$. We have $\hat{S}^p_h = \hat{S}^p_{h_s} \otimes \hat{S}^p_{h_t} = \hat{S}^p_{h_s} \otimes \cdots \otimes \hat{S}^p_{h_s} \otimes \hat{S}^p_{h_t}$, where

$$\hat{S}^p_{h_s} := \left\{ \hat{B}_{i,s,h}(\eta) \mid i_k = 1, \ldots, m_k \text{ for } k = 1, \ldots, d \right\}.$$ 

The minimum regularity of the spline spaces that we assume is the following.

**Assumption 2.** We assume that $p_s \geq 2$, $\hat{S}^p_{h_s} \subset C^1(\hat{\Omega})$, $p_t \geq 1$ and $\hat{S}^p_{h_t} \subset C^0(\hat{\Omega})$.

### 2.2 Isogeometric spaces

The space domain $\Omega \subset \mathbb{R}^d$ is given as a spline non-singular single-patch, that is, the following conditions are fulfilled.

**Assumption 3.** We assume that $F : \hat{\Omega} \to \Omega$, with $F \in \hat{S}^p_{h_s}$ on the closure of $\Omega$.

**Assumption 4.** We assume that $F^{-1}$ has piecewise bounded derivatives of any order.

Let $x = (x_1, \ldots, x_d) := F(\eta)$. Given $T > 0$, the space-time computational domain $\Omega \times [0, T]$ is given by the parametrization $G \in \hat{S}^p_{h_s} \otimes \hat{S}^p_{h_t}$ such that $G : [0, T] \times [0, 1] \to \Omega \times [0, T]$ with $G(\eta, \tau) := (F(\eta), T\tau) = (x, t)$, and where $t := T\tau$. We introduce, in the parametric domain, the space with boundary conditions

$$\hat{\nu}_{h,0} := \left\{ \hat{\nu}_h \in \hat{S}^p_h \mid \hat{\nu}_h = 0 \text{ on } \partial \hat{\Omega} \times [0,1] \text{ and } \hat{\nu}_h = 0 \text{ on } \hat{\Omega} \times \{0\} \right\}.$$ 

Note that $\hat{\nu}_{h,0} = \hat{\nu}_{h,0} \otimes \hat{\nu}_{h,t,0}$, where

$$\hat{\nu}_{s,h,0} := \left\{ \hat{\nu}_h \in \hat{S}^p_{h_s} \mid \hat{\nu}_h = 0 \text{ on } \partial \hat{\Omega} \right\} = \left\{ \hat{b}_{i_1,p_1} \cdots \hat{b}_{i_d,p_d} \mid i_k = 2, \ldots, m_k - 1; k = 1, \ldots, d \right\},$$

$$\hat{\nu}_{t,h,0} := \left\{ \hat{\nu}_h \in \hat{S}^p_{h_t} \mid \hat{\nu}_h(0) = 0 \right\} = \left\{ \hat{b}_{i_t,p_t} \mid i_t = 2, \ldots, m_t \right\}. \quad (1a)$$

Reordering the basis and then introducing the colexicographical ordering of the degrees-of-freedom, we have

$$\hat{\nu}_{s,h,0} = \left\{ \hat{b}_{i_1,p_1} \cdots \hat{b}_{i_d,p_d} \mid i_k = 1, \ldots, n_{s,k}; k = 1, \ldots, d \right\} = \left\{ \hat{B}_{i,p} \mid i = 1, \ldots, N_s \right\},$$

$$\hat{\nu}_{t,h,0} = \left\{ \hat{b}_{i_t,p_t} \mid i = 1, \ldots, n_t \right\}. \quad (1b)$$
and
\[ \tilde{V}_{h,0} = \text{span} \left\{ \tilde{B}_{i,p} \mid i = 1, \ldots, N_{dof} \right\}, \]

where we have defined
\[ n_t := m_t - 1, \quad N_s := \prod_{k=1}^{d} n_{s,k}, \quad n_{s,k} := m_k - 1, \quad N_{dof} := N_s/n_t. \]

The isogeometric space we consider is the isoparametric push-forward of \( \tilde{V}_{h,0} \), i.e.
\[ V_{h,0} := \text{span} \left\{ B_{i,p} := \tilde{B}_{i,p} \circ \mathbf{G}^{-1} \mid i = 1, \ldots, N_{dof} \right\}. \]

Note that \( V_{h,0} \) can be written as
\[ V_{h,0} = V_{s,h,0} \otimes V_{t,h,0}, \]

where
\[ V_{s,h,0} := \text{span} \left\{ B_{i,p_s} := \tilde{B}_{i,p_s} \circ \mathbf{F}^{-1} \mid i = 1, \ldots, N_s \right\}, \quad V_{t,h,0} := \text{span} \left\{ b_{i,p_t} := \tilde{b}_{i,p_t}(\cdot,T) \mid i = 1, \ldots, n_t \right\}. \]

## 3 Parabolic model problem and its discretization

We denote by \( \partial_t \) the partial time derivative and by \( \Delta \) the laplacian w.r.t. spatial variables. If \( A \) and \( B \) are Hilbert spaces, \( A \otimes B \) denotes the closure of their tensor product (see [2, Definition 12.3.2]). We also identify the spaces \( H^m((0,T);H^n(\Omega)), H^m(\Omega) \otimes H^m(0,T) \) and \( H^m(\Omega \times (0,T)) \), (see [2, Section 12.7]).

The functional framework we employ is provided by the Hilbert space
\[ V_0 := \left\{ v \in \left[ H\Delta(\Omega) \otimes L^2(0,T) \right] \cap \left[ L^2(\Omega) \otimes H^1(0,T) \right] \mid v = 0 \text{ on } \Omega \times \{0\} \right\}, \]

where \( H\Delta(\Omega) := \{ w \in H^1_0(\Omega) \mid \Delta w \in L^2(\Omega) \} \). The space above is endowed with the norm
\[ \|v\|_{V_0}^2 := \|v\|_{H\Delta(\Omega)\otimes L^2(0,T)}^2 + \|v\|_{L^2(\Omega)\otimes H^1(0,T)}^2 = \int_0^T \|\Delta v\|_{L^2(\Omega)}^2 \, dt + \int_0^T \|\partial_t v\|_{L^2(\Omega)}^2 \, dt. \]

**Remark 1.** Thanks to Assumption 3, \( \Omega \) has a piecewise smooth boundary with bounded curvature. Recalling [19, Lemma 11.1], \( H^1_0(\Omega) \cap H^2(\Omega) \) is then a closed subspace of \( H\Delta(\Omega) \), that is, there exists a constant \( C > 0 \) depending only on the space parametrization \( \mathbf{F} \) such that
\[ \|v\|^2_{H^1_0(\Omega)} \leq C\|\Delta v\|^2_{L^2(\Omega)} \quad \forall v \in H^1_0(\Omega) \cap H^2(\Omega). \]

Our model problem is the heat equation, with initial and homogeneous boundary conditions: we seek for a solution \( u \) such that
\[ \begin{cases} \partial_t u - \Delta u = f & \text{in } \Omega \times (0,T), \\ u = 0 & \text{on } \partial\Omega \times (0,T), \\ u = 0 & \text{in } \Omega \times \{0\}. \end{cases} \]

We assume that \( f \in L^2(\Omega \times (0,T)) \). Thanks to Assumptions 3–4, there exists a unique solution \( u \) such that
\[ u \in H^2(\Omega) \otimes L^2(0,T) \cap L^2(\Omega) \otimes H^1(0,T) \]

of the problem (5), see Appendix A.1.

More generally, non-homogeneous initial and boundary conditions are allowed. For example, if \( u = u_0 \) at \( \Omega \times \{0\} \), introducing a suitable lifting \( \tilde{u}_0 \in H^2(\Omega) \otimes L^2(0,T) \cap L^2(\Omega) \otimes H^1(0,T) \) of \( u_0 \neq 0 \), then \( \tilde{u} = u - \tilde{u}_0 \in V_0 \) is the solution of
\[ \begin{cases} \tilde{\partial}_t \tilde{u} - \Delta \tilde{u} = \tilde{f} & \text{in } \Omega \times (0,T), \\ \tilde{u} = 0 & \text{on } \partial\Omega \times (0,T), \\ \tilde{u} = 0 & \text{in } \Omega \times \{0\}, \end{cases} \]

where \( \tilde{f} := f - \partial_t \tilde{u}_0 + \Delta \tilde{u}_0 \). For a detailed description of the variational formulation of problems (5)–(7) and their well-posedness see, for example, [11, 27].
3.1 Variational formulation

We consider a non-standard variational formulation for the system (5) which is motivated by its next discretization in Section 3.2. It reads: find \( u \in V_0 \) such that

\[
    u = \arg \min_{v \in V_0} \frac{1}{2} \| \partial_t v - \Delta v - f \|^2_{L^2(\Omega \times (0,T))}.
\]  

(8)

Its Euler-Lagrange equation is

\[
    \mathcal{A}(u, v) = \mathcal{F}(v) \quad \forall v \in V_0,
\]  

(9)

where the bilinear form \( \mathcal{A}(\cdot, \cdot) \) and the linear form \( \mathcal{F}(\cdot) \) are defined as

\[
    \mathcal{A}(v, w) := \int_0^T \int_\Omega (\partial_t v \partial_t w + \Delta v \Delta w - \partial_t \Delta w - \Delta \partial_t w) \, d\Omega \, dt,
\]

\[
    \mathcal{F}(w) := \int_0^T \int_\Omega f (\partial_t w - \Delta w) \, d\Omega \, dt.
\]

For an equivalent way of writing the minimization problem (8), we refer to Appendix A.2.

The variational formulation (9) is well-posed, thanks to the following Lemmas 1–3 and Proposition 1.

Lemma 1. The bilinear form \( \mathcal{A}(\cdot, \cdot) \) is continuous in \( V_0 \). In particular it holds

\[
    |\mathcal{A}(v, w)| \leq 2 \|v\|_{V_0} \|w\|_{V_0} \quad \forall v, w \in V_0.
\]

Proof. Given \( v, w \in V_0 \), by Cauchy-Schwarz inequality

\[
    |\mathcal{A}(v, w)| \leq \|v\|_{V_0} \|w\|_{V_0} + \int_0^T \int_\Omega (|\partial_t v \Delta w| + |\Delta v \partial_t w|) \, d\Omega \, dt
\]

\[
    \leq \|v\|_{V_0} \|w\|_{V_0} + \left[ \int_0^T \left( \|\partial_t v \|^2_{L^2(\Omega)} + \|\Delta v \|^2_{L^2(\Omega)} \right) \, dt \right]^{1/2} \left[ \int_0^T \left( \|\partial_t w \|^2_{L^2(\Omega)} + \|\Delta w \|^2_{L^2(\Omega)} \right) \, dt \right]^{1/2}
\]

\[
    \leq 2 \|v\|_{V_0} \|w\|_{V_0},
\]

which concludes the proof.

Lemma 2. The bilinear form \( \mathcal{A}(\cdot, \cdot) \) is \( V_0 \)-elliptic. In particular, it holds

\[
    \mathcal{A}(v, v) \geq \|v\|^2_{V_0} \quad \forall v \in V_0.
\]

Proof. Let \( v \in V_0 \). Thanks to [6, Lemma 3.3], we can write

\[
    -2 \int_0^T \int_\Omega \partial_t v \Delta v \, d\Omega \, dt = \int_\Omega |\nabla v(x, T)|^2 \, d\Omega - \int_\Omega |\nabla v(x, 0)|^2 \, d\Omega,
\]

where \( \nabla := [\partial_{x_1}, \ldots, \partial_{x_d}]^T \) denotes the gradient w.r.t. spatial variables \( x_1, \ldots, x_d \). In particular, as \( \nabla v(x, 0) = 0 \), we have that

\[
    \mathcal{A}(v, v) = \int_0^T \|\partial_t v\|^2_{L^2(\Omega)} \, dt + \int_0^T \|\Delta v\|^2_{L^2(\Omega)} \, dt + \int_\Omega |\nabla v(x, T)|^2 \, d\Omega \geq \|v\|^2_{V_0} \quad \forall v \in V_0,
\]

which concludes the proof.

Lemma 3. The linear form \( \mathcal{F}(\cdot) \) is continuous in \( V_0 \). In particular it holds

\[
    \mathcal{F}(v) \leq \sqrt{2} \|f\|_{L^2(\Omega \times (0,T))} \|v\|_{V_0} \quad \forall v \in V_0.
\]
Proof. Given \( v \in V_0 \), by Cauchy-Schwarz inequality we get
\[
|F(v)| \leq \|f\|_{L^2(\Omega \times (0,T))} \left( \int_0^T \| \partial_t v - \Delta v \|_{L^2(\Omega)}^2 \, dt \right)^{1/2}
\]
\[
\leq \sqrt{2} \|f\|_{L^2(\Omega \times (0,T))} \left( \int_0^T \| \partial_t v \|_{L^2(\Omega)}^2 \, dt + \int_0^T \| \Delta v \|_{L^2(\Omega)}^2 \, dt \right)^{1/2}
\]
\[
= \sqrt{2} \|f\|_{L^2(\Omega \times (0,T))} \|v\|_{V_0},
\]
which concludes the proof. \( \square \)

**Proposition 1.** The minimization problem (8) and the variational problem (9) are equivalent and they admit a unique solution \( u \in V_0 \).

**Proof.** The proof follows using Lemmas 1–3 and the Lax-Milgram theorem. \( \square \)

### 3.2 Least-squares approximation

Thanks to Assumption 2, we have
\[
V_h,0 \subset (H^1_0(\Omega) \cap H^2(\Omega)) \otimes H^1(0,T) \subset V_0.
\] (10)

Therefore we consider a Galerkin method for (9), that is, the least-squares approximation of the system (5): find \( u_h \in V_h,0 \) such that
\[
u_h = \arg \min_{v_h \in V_h,0} \frac{1}{2} \| \partial_t v_h - \Delta v_h - f \|_{L^2(\Omega \times (0,T))}^2.
\] (11)

Its Euler-Lagrange equation is
\[
A(u_h, v_h) = F(v_h) \quad \forall v_h \in V_h,0.
\] (12)

Well-posedness and quasi-optimality follow from standard arguments.

**Proposition 2.** The minimization problem (11) and the variational problem (12) are equivalent and they admit a unique solution \( u_h \in V_h,0 \). It also holds:
\[
\|u - u_h\|_{V_0} \leq \sqrt{2} \inf_{v_h \in V_h,0} \|u - v_h\|_{V_0}.
\] (13)

**Proof.** The proof of the equivalence and of the existence and uniqueness of a solution follow by using Lemmas 1–3 and the Lax-Milgram theorem, while the proof of (13) is a consequence of the Céa Lemma and the symmetry of the bilinear form \( A \). \( \square \)

**Remark 2.** Thanks to (6) and (10), we have that \( \inf_{v_h \in V_h,0} \|u - v_h\|_{V_0} \) goes to zero as \( h \to 0 \), that is, the least-squares approximation (11) is convergent.

### 3.3 A priori error analysis

We investigate in this section the approximation properties of the isogeometric space \( V_{h,0} \) under \( h \)-refinement.

**Proposition 3.** Let \( q_s \) and \( q_t \) be two integers such that \( 2 \leq q_s \leq p_s + 1 \) and \( 1 \leq q_t \leq p_t + 1 \). Under Assumption 1, there exists a projection \( \Pi_h : V_0 \cap (H^{q_s}(\Omega) \otimes L^2(0,T)) \cap (L^2(\Omega) \otimes H^{q_t}(0,T)) \to V_{h,0} \) such that
\[
\|u - \Pi_h v\|_{V_0} \leq C \left( h_{\Omega}^{q_s - 2} \|v\|_{H^{q_s}(\Omega) \otimes L^2(0,T)} + h_{t}^{q_t - 1} \|v\|_{L^2(\Omega) \otimes H^{q_t}(0,T)} \right)
\] (14)

where the constant \( C \) depends on \( p_s, p_t, \alpha \) and the parametrization \( G \).
**Proof.** The result follows from the anisotropic approximation estimates that are developed in [5]. We remark that [5] states its error analysis in dimension 2, but the results therein straightforwardly generalize to higher dimension. We give an overview of the proof, for the sake of completeness.

As space and time coordinates in \( \Omega \times [0,T] \) are orthogonal, the parametric coordinate (tangent) vectors are

\[
g_i(x) := \partial_n G \circ G^{-1}(x,t) = \begin{bmatrix} \partial_n F \circ F^{-1}(x) \\ 0 \end{bmatrix} \in \mathbb{R}^d \times \{0\} \subset \mathbb{R}^{d+1} \quad \text{for } i = 1, \ldots, d,
\]

\[
g_t(t) := \partial_t G \circ G^{-1}(x,t) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ T \end{bmatrix} \in \mathbb{R}^{d+1}.
\]

Then, given \( v \in V_0 \), the directional derivatives w.r.t. \( g_i \) and \( g_t \) that are used in [5, Section 5], become

\[
\frac{\partial v}{\partial g_i}(x,t) = (J_F \circ F^{-1}(x))^T \nabla v(x,t), \quad \frac{\partial v}{\partial g_t}(x,t) = T \partial_t v(x,t).
\]

Higher-order directional derivatives can be defined similarly, as in [5, Section 5]. We also have that

\[
\left\| \frac{\partial}{\partial g_i} \left( \cdots \frac{\partial v}{\partial g_i} \right) \right\|_{L^2(\Omega \times (0,T))} \leq C \|v\|_{H^k(\Omega) \otimes L^2(0,T)},
\]

\[
\left\| \frac{\partial^k v}{\partial t^k} \right\|_{L^2(\Omega \times (0,T))} \leq C \|v\|_{L^2(\Omega) \otimes H^k(0,T)},
\]

for a suitable constant \( C, k \geq 0 \) and \( i_j \in \{1, \ldots, d\} \), \( j = 1, \ldots, k \). Therefore, [5, Theorem 5.1] generalized to \( d + 1 \) dimensions gives the existence of a projection \( \Pi_h : V_0 \to V_{h,0} \) such that

\[
\|v - \Pi_h v\|_{H^2(\Omega) \otimes L^2(0,T)} \leq C \left( h^{k_s-2}_s \|v\|_{H^{q_s}(\Omega) \otimes L^2(0,T)} + h^{k_t}_t \|v\|_{H^2(\Omega) \otimes H^{q_t}(0,T)} \right),
\]

\[
\|v - \Pi_h v\|_{L^2(\Omega) \otimes H^{q_t}(0,T)} \leq C \left( h^{k_t}_t \|v\|_{H^{q_t}(\Omega) \otimes H^{q_s}(0,T)} + h^{k_s-1}_s \|v\|_{L^2(\Omega) \otimes H^{q_s}(0,T)} \right),
\]

with \( C \) depending only on \( p_s, p_t, \alpha \) and the space parametrization \( G \). Squaring and summing the two inequalities above, using (15) and that \( \|v - \Pi_h v\|_{H^s(\Omega) \otimes L^2(0,T)} \leq \|v - \Pi_h v\|_{H^2(\Omega) \otimes L^2(0,T)} \), we finally get (14).

As a direct corollary of Proposition 2 and 3, we can now state the a-priori error estimate for the least-squares method.

**Theorem 1.** Let \( q_s \) and \( q_t \) be two integers such that \( q_s \geq 2 \) and \( q_t \geq 1 \). If \( u \in V_0 \cap (H^{q_s}(\Omega) \otimes L^2(0,T)) \cap (L^2(\Omega) \otimes H^{q_t}(0,T)) \) is the solution of (5) and \( u_h \in V_{h,0} \) is the solution of (12), then

\[
\|u - u_h\|_{V_0} \leq C(h^{k_s-2}_s \|u\|_{H^{q_s}(\Omega) \otimes L^2(0,T)} + h^{k_t}_t \|u\|_{L^2(\Omega) \otimes H^{q_t}(0,T)}\)
\]

where \( k_s := \min\{q_s, p_s + 1\} \), \( k_t := \min\{q_t, p_t + 1\} \), \( C \) is a constant that depends only on \( p_s, p_t, \alpha \) and the parametrization \( G \).

## 4 Linear solver

In this section we analyze solving strategies for the least-squares method (12) and we present a suitable preconditioner.

We recall that the Kronecker product between two matrices \( C \in \mathbb{R}^{n_c \times n_c} \) and \( D \in \mathbb{R}^{n_d \times n_d} \) is defined as

\[
C \otimes D := \begin{bmatrix} [C]_{11} D & \ldots & [C]_{1n_c} D \\ \vdots & \ddots & \vdots \\ [C]_{n_c 1} D & \ldots & [C]_{n_c n_d} D \end{bmatrix} \in \mathbb{R}^{n_c n_d \times n_c n_d},
\]

where \([C]_{ij}\) denotes the \( ij \)-th entry of the matrix \( C \). We will use the following properties (see [17]):
• it holds
  \[(C \otimes D)^T = C^T \otimes D^T;\]  \hfill (17)

• if \(C, D, E\) and \(F\) are matrices and there exist the products \(CE\) and \(DF\), it holds
  \[(C \otimes D) \cdot (E \otimes F) = (CE) \otimes (DF);\]  \hfill (18)

• if \(C\) and \(D\) are non-singular, then
  \[(C \otimes D)^{-1} = C^{-1} \otimes D^{-1};\]  \hfill (19)

• if \(X \in \mathbb{R}^{n_x \times n_x}\) then
  \[(C \otimes D)\text{vec}(X) = \text{vec}(DXC^T)\]  \hfill (20)

  where the “\text{vec}” operator stacks the columns of a matrix in a vector.

4.1 Discrete system

Before introducing the discrete system, we rewrite the bilinear form \(\mathcal{A}(\cdot, \cdot)\) in an equivalent way, through the following Lemma.

**Lemma 4.** The bilinear form \(\mathcal{A}(\cdot, \cdot)\) can be written as

\[
\mathcal{A}(v_h, w_h) = \int_0^T \int_\Omega \partial_t v_h \partial_t w_h \, d\Omega \, dt + \int_0^T \int_\Omega \Delta v_h \Delta w_h \, d\Omega \, dt + \int_\Omega \nabla v_h(x, T) \cdot \nabla w_h(x, T) \, d\Omega \tag{21}
\]

for all \(v_h, w_h \in \mathcal{V}_{h,0}\).

**Proof.** Let \(v_h, w_h \in \mathcal{V}_{h,0}\). First note that \(\partial_t v_h, \partial_t w_h \in (H^1_x(\Omega) \cap H^2(\Omega)) \otimes L^2(0, T)\), from (10), and \(\partial_t v_h = \partial_t w_h = 0\) on \(\partial \Omega \times [0, T]\). Using Green formula and integrating by parts yields to

\[
- \int_0^T \int_\Omega (\partial_t v_h \Delta w_h + \partial_t w_h \Delta v_h) \, d\Omega \, dt = - \int_0^T \int_\partial \Omega (\partial_t v_h \nabla w_h \cdot \nu + \partial_t w_h \nabla v_h \cdot \nu) \, d\Omega \, dt
\]

\[
+ \int_0^T \int_\Omega [\nabla(\partial_t v_h) \cdot \nabla w_h + \nabla(\partial_t w_h) \cdot \nabla v_h] \, d\Omega \, dt
\]

\[
= \int_0^T \left[ \partial_t \left( \int_\Omega \nabla v_h \cdot \nabla w_h \, d\Omega \right) \right] \, dt
\]

\[
= \int_\Omega \nabla v_h(x, T) \cdot \nabla w_h(x, T) - \nabla v_h(x, 0) \cdot \nabla w_h(x, 0) \, d\Omega
\]

where \(\nu \in \mathbb{R}^d\) is the external normal unit vector to \(\partial \Omega\). Then (21) follows. \(\square\)

After the introduction of the basis (3) for \(\mathcal{V}_{h,0}\), the linear system associated to (12) is

\[
Au = F
\]

where \([A]_{ij} := \mathcal{A}(B_{i,p}, B_{j,p})\) and \([F]_i := \mathcal{F}(B_{i,p})\). The discrete system matrix \(A\) can be written as the sum of Kronecker product matrices (see (21))

\[
A = K_t \otimes M_s + M_t \otimes J_s + W_t \otimes L_s \tag{22}
\]

where the time matrices are for \(i, j = 1, \ldots, n_t\)

\[
[K_t]_{ij} := \int_0^T b_{i,p}(t) b_{j,p}(t) \, dt, \quad [M_t]_{ij} := \int_0^T b_{i,p}(t) b_{j,p}(t) \, dt, \quad [W_t]_{ij} := b_{i,p}(T) b_{j,p}(T),
\]

and the spatial matrices are for \(i, j = 1, \ldots, N_s\)

\[
[J_s]_{ij} := \int_\Omega \Delta B_{i,p}(x) \Delta B_{j,p}(x) \, d\Omega, \quad [M_s]_{ij} := \int_\Omega B_{i,p}(x) B_{j,p}(x) \, d\Omega,
\]

\[
[L_s]_{ij} := \int_\Omega \nabla B_{i,p}(x) \nabla B_{j,p}(x) \, d\Omega.
\]
4.2 Preconditioner definition and properties

The matrix $A$ in (22) is symmetric and positive definite. Thus we design and analyze a suitable symmetric positive definite preconditioners to be used for a preconditioned Conjugate Gradient method.

The simpler version of our preconditioner is associated with the bilinear form $\widehat{P} : V_{h,0} \times V_{h,0} \to \mathbb{R}$ defined as

$$\widehat{P}(w_h, v_h) := \int_0^1 \int_{\hat{\Omega}} \partial_\tau w_h \partial_\tau v_h \, d\hat{\Omega} \, d\tau + \sum_{k=1}^d \int_0^1 \int_{\hat{\Omega}} \frac{\partial^2 w_h}{\partial \eta_k^2} \frac{\partial^2 v_h}{\partial \eta_k^2} \, d\hat{\Omega} \, d\tau$$

(23)

and with the corresponding norm

$$\|v_h\|_{\widehat{P}}^2 := \widehat{P}(v_h, v_h).$$

(24)

The preconditioner matrix is given by

$$[P]_{ij} = \widehat{P}(\hat{B}_{i,p}(\eta, \tau), \hat{B}_{j,p}(\eta, \tau)) \quad i, j = 1, \ldots, N_{dof}$$

and has the following structure:

$$P = \hat{K}_t \otimes \hat{M}_s + \hat{M}_t \otimes \hat{J}_s,$$

(25)

where, referring to (1) for the notation of the basis functions,

$$[\hat{K}_t]_{ij} := \int_0^1 \hat{b}_{i,p}(\tau) \hat{b}_{j,p}(\tau) \, d\tau, \quad [\hat{M}_t]_{ij} := \int_0^1 \hat{b}_{i,p}(\tau) \hat{\theta}_{j,p}(\tau) \, d\tau \quad i, j = 1, \ldots, n_t,$$

$$[\hat{J}_s]_{ij} := \sum_{k=1}^d \int_{\hat{\Omega}} \frac{\partial^2 \hat{B}_{i,p}(\eta)}{\partial \eta_k^2} \frac{\partial^2 \hat{B}_{j,p}(\eta)}{\partial \eta_k^2} \, d\hat{\Omega}, \quad [\hat{M}_s]_{ij} := \int_{\hat{\Omega}} \hat{B}_{i,p}(\eta) \hat{B}_{j,p}(\eta) \, d\hat{\Omega} \quad i, j = 1, \ldots, N_s.$$

Note that $\hat{K}_t$, $\hat{M}_t$ and $\hat{M}_s$ correspond to $K_t$, $M_t$ and $M_s$, respectively, where the integration is performed on the parametric domain $\hat{\Omega}$. The matrices $\hat{J}_s$ and $\hat{M}_s$ can be further factorized as sum of Kronecker products as

$$\hat{J}_s = \sum_{k=1}^d \hat{M}_d \otimes \cdots \otimes \hat{M}_{k+1} \otimes \hat{J}_k \otimes \hat{M}_{k-1} \otimes \cdots \otimes \hat{M}_1, \quad \hat{M}_s = \hat{M}_d \otimes \cdots \otimes \hat{M}_1,$$

where for $k = 1, \ldots, d$

$$[\hat{J}_s]_{ij} := \int_0^1 \hat{b}_{i,p}(\eta_k) \hat{b}_{j,p}(\eta_k) \, d\eta_k, \quad [\hat{M}_s]_{ij} := \int_0^1 \hat{b}_{i,p}(\eta_k) \hat{b}_{j,p}(\eta_k) \, d\eta_k \quad i, j = 1, \ldots, n_{s,k}.$$

If $d = 3$, that is the case addressed in the numerical tests, we have that (25) becomes

$$P = \hat{K}_t \otimes \hat{M}_3 \otimes \hat{M}_2 \otimes \hat{M}_1 + \hat{M}_t \otimes \hat{J}_3 \otimes \hat{M}_2 \otimes \hat{M}_1 + \hat{M}_t \otimes \hat{M}_3 \otimes \hat{J}_2 \otimes \hat{M}_1 + \hat{M}_t \otimes \hat{M}_3 \otimes \hat{M}_2 \otimes \hat{J}_1.$$

4.2.1 Spectral analysis

We now focus on the spectral analysis of $P^{-1}A$. We need to define the bilinear form $\mathcal{P} : V_{h,0} \times V_{h,0} \to \mathbb{R}$

$$\mathcal{P}(w_h, v_h) := \int_{0}^{T} \int_{\Omega} \partial_\tau w_h \partial_\tau v_h \, d\Omega \, dt + \sum_{k=1}^d \int_{0}^{T} \int_{\Omega} \frac{\partial^2 w_h}{\partial x_k^2} \frac{\partial^2 v_h}{\partial x_k^2} \, d\Omega \, dt$$

and the associated norm

$$\|v_h\|_{\mathcal{P}}^2 := \mathcal{P}(v_h, v_h).$$

Note that $\mathcal{P}(\cdot, \cdot)$ and $\|\cdot\|_{\mathcal{P}}$ are analogous to $\widehat{P}(\cdot, \cdot)$ and $\|\cdot\|_{\widehat{P}}$ but integration is performed on the physical domain (see (23) and (24)).

We first prove the equivalence between the norms $\|\cdot\|_{\mathcal{P}}$ and $\|\cdot\|_{v_h}$ in $V_{h,0}$.
Proposition 4. It holds
\[ \frac{1}{C} \|v_h\|_F^2 \leq \|v_h\|_{V_0}^2 \leq d\|v_h\|_F^2 \quad \forall v_h \in V_{h,0}, \]
where $C$ is the constant defined in (4).

Proof. Given $v_h \in V_{h,0}$, recalling (10) and thanks to (4), we have that
\[ \sum_{k=1}^d \int_0^T \int_{\Omega} \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|^2 \, d\Omega \, dt \leq \int_0^T \int_{\Omega} \left( \sum_{k,l=1}^d \left| \frac{\partial^2 v_h}{\partial x_k \partial x_l} \right|^2 \right) \, d\Omega \, dt = \int_0^T \|v_h\|_{H^2(\Omega)}^2 \, dt \]
\[ \leq \int_0^T \|v_h\|_{H^2(\Omega)}^2 \, dt \leq C \int_0^T \|\Delta v_h\|_{L^2(\Omega)}^2 \, dt. \]

Thus, the first inequality holds. We also have
\[ \int_0^T \|\Delta v_h\|_{L^2(\Omega)}^2 \, dt = \sum_{k,l=1}^d \int_0^T \int_{\Omega} \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|^2 \, d\Omega \, dt \leq \frac{1}{2} \sum_{k,l=1}^d \int_0^T \left[ \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|_{L^2(\Omega)}^2 + \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|_{L^2(\Omega)}^2 \right] \, dt \]
\[ \leq d \sum_{k=1}^d \int_0^T \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|_{L^2(\Omega)}^2 \, dt = d \sum_{k=1}^d \int_0^T \int_{\Omega} \left| \frac{\partial^2 v_h}{\partial x_k^2} \right|^2 \, d\Omega \, dt \]
and we can conclude that the second inequality holds. \qed

Corollary 1. It holds
\[ \frac{1}{C} \|v_h\|_F^2 \leq A(v_h, v_h) \leq 2d\|v_h\|_F^2 \quad \forall v_h \in V_{h,0}. \]

Proof. The statement follows from Lemma 1, Lemma 2 and Proposition 4. \qed

Proposition 5. There exist constants $Q_1, Q_2 > 0$ independent of $h_s, h_t, p_s, p_t$, but dependent on $G$ such that
\[ Q_1 \|v_h\|_F^2 \leq \|\hat{v}_h\|_F^2 \leq Q_2 \|v_h\|_F^2 \quad \forall v_h \in \hat{V}_{h,0} \text{ and } v_h := \hat{v}_h \circ G^{-1}. \]

Proof. Let $\hat{v}_h \in \hat{V}_{h,0}$ and $v_h := \hat{v}_h \circ G^{-1} \in V_{h,0}$. First we prove the first inequality. Observing that $G^{-1}(x, t) = (F^{-1}(x), t/T)$, we get
\[ \int_0^T \int_{\Omega} (\partial_t v_h)^2 \, d\Omega \, dt = \frac{1}{T} \int_0^1 \int_{\Omega} (\partial_t \hat{v}_h)^2 \, d\Omega \, d\tau \leq \frac{1}{T} \sup_{\Omega} (|\det(J_F)|) \int_0^1 \|\partial_t \hat{v}_h\|_{L^2(\Omega)}^2 \, d\tau \]
\[ \leq \frac{1}{T} \sup_{\Omega} (|\det(J_F)|) \|\hat{v}_h\|_F^2. \]

Let $\mathbb{H}_{\hat{v}_h}$ be the Hessian of $\hat{v}_h$ with respect to the spatial parametric variables $\eta_1, \ldots, \eta_d$, i.e. $\mathbb{H}_{\hat{v}_h} \in \mathbb{R}^{d \times d}$ with $[\mathbb{H}_{\hat{v}_h}]_{ij} = \frac{\partial^2 \hat{v}_h}{\partial \eta_i \partial \eta_j}$ for $i, j = 1, \ldots, d$, and let $[J_F^{-1}]_{,i} \in \mathbb{R}^d$ denote the $i$-th column of $J_F^{-1}$. Then, for $i = 1, \ldots, d$, it holds
\[ \int_0^T \int_{\Omega} \left( \frac{\partial^2 v_h}{\partial x_i^2} \right)^2 \, d\Omega \, dt = \int_0^1 \int_{\Omega} \left( [J_F^{-1}]_{i} \mathbb{H}_{\hat{v}_h} [J_F^{-1}]_{,i} + \nabla \hat{v}_h \frac{\partial [J_F^{-1}]_{,i}}{\partial \eta_i} \right)^2 T |\det(J_F)| \, d\Omega \, d\tau \]
\[ \leq \int_0^1 \int_{\Omega} \hat{C}_1 \|\mathbb{H}_{\hat{v}_h}\|_F^2 + \hat{C}_2 \|
abla \hat{v}_h\|_F^2 \, d\Omega \, d\tau, \]

where $\| \cdot \|_F$ and $\| \cdot \|_2$ denote the Frobenius norm and the norm two of matrices, respectively. Then, \[ \hat{C}_1 := 2T \max_{\Omega} \sup_{\eta} \left\{ \left( \left[ [J_F^{-1}]_{,i} \right]_2^2 |\det(J_F)| \right) \right\} \] and \[ \hat{C}_2 := 2T \max_{\Omega} \sup_{\eta} \left\{ \left( \left[ \frac{\partial [J_F^{-1}]_{,i}}{\partial \eta_i} \right]_2 \right) \right\} \] and where we used that $\|\mathbb{H}_{\hat{v}_h}\|_2 \leq \|\mathbb{H}_{\hat{v}_h}\|_F$. \qed
Following the proof of Proposition 4, we can prove that

$$\int_0^1 \| \Delta \tilde{v}_h \|^2_{L^2(\Omega)} \, d\tau \leq d \| \tilde{v}_h \|^2_{P} \quad \forall \tilde{v}_h \in \hat{V}_{h,0}.$$ 

Thus it holds

$$\int_0^1 \int_{\Omega} |\tilde{v}_h|^2 \, d\Omega \, d\tau \leq 2 \int_0^1 \| \tilde{v}_h \|^2_{H^2(\Omega)} \, d\tau \leq 2\tilde{C} \int_0^1 \| \Delta \tilde{v}_h \|^2_{L^2(\Omega)} \, d\tau \leq 2d\tilde{C} \| \tilde{v}_h \|^2_{P},$$

$$\int_0^1 \int_{\Omega} |\nabla \tilde{v}_h|^2 \, d\Omega \, d\tau = \int_0^1 \| \tilde{v}_h \|^2_{H^1(\Omega)} \, d\tau \leq \tilde{C} \int_0^1 \| \Delta \tilde{v}_h \|^2_{L^2(\Omega)} \, d\tau \leq d\tilde{C} \| \tilde{v}_h \|^2_{P},$$

where $\tilde{C} > 0$ is the constant such that $\| v \|^2_{H^2(\Omega)} \leq \tilde{C} \| \Delta v \|^2_{L^2(\Omega)}$, for $v \in H^1_0(\Omega) \cap H^2(\Omega)$. Therefore, we have

$$\int_0^T \int_{\Omega} \left( \frac{\partial^2 v_h}{\partial x_i^2} \right)^2 \, d\Omega \, dt \leq d\tilde{C} \left( 2\tilde{C}_1 + \tilde{C}_2 \right) \| v_h \|^2_{P}$$

and, summing all terms that define $\| \cdot \|_P$, we conclude

$$Q_1 \| v_h \|^2_{P} \leq \| \tilde{v}_h \|^2_{P}$$

with $\frac{1}{Q_1} := \frac{1}{d} \sup_{\Omega} \{ |\det(J_F)| \} + d\tilde{C} \left( 2\tilde{C}_1 + \tilde{C}_2 \right)$.

Now we prove the other bound. We observe that $\tilde{v}_h = v_h \circ G$ and $G(\eta, \tau) = (F(\eta), T\tau)$. Thus, with similar arguments and using (4), we have

$$\int_0^1 \int_{\Omega} \partial_t \tilde{v}_h^2 \, d\Omega \, d\tau \leq T \sup_{\Omega} \{ |\det(J_{F^{-1}})| \} \| v_h \|^2_{P} \quad \text{and} \quad \int_0^1 \int_{\Omega} \left( \frac{\partial^2 \tilde{v}_h}{\partial \eta^2} \right)^2 \, d\Omega \, d\tau \leq d\tilde{C} (2C_1 + C_2) \| v_h \|^2_{P},$$

where $C_1 := 2\frac{1}{\tau} \max_i \sup_{\Omega} \left\{ \left( \| [J_{F^{-1}}] \| \right)^2 \right\}$ and $C_2 := 2\frac{1}{\tau} \max_i \sup_{\Omega} \left\{ \left( \| [J_{F^{-1}}] \| \right)^2 \right\}$.

We conclude that

$$\| \tilde{v}_h \|^2_{P} \leq Q_2 \| v_h \|^2_{P}$$

with $Q_2 := T \sup_{\Omega} \{ |\det(J_{F^{-1}})| \} + d\tilde{C} (2C_1 + C_2)$.

\begin{proof}

\textbf{Theorem 2.} It holds

$$\theta \leq \lambda_{\min}(P^{-1}A), \quad \lambda_{\max}(P^{-1}A) \leq \Theta,$$

where $\theta$ and $\Theta$ are positive constants that do not depend on $h_x, h_t, p_x$, and $p_t$.

\textbf{Proof.} Let $\tilde{v}_h \in \hat{V}_{h,0}$, $v$ its coordinate vector with respect to the basis (2) and $v_h = \tilde{v}_h \circ G^{-1} \in V_{h,0}$. Thanks to Courant-Fischer theorem, we need to find $\theta$ and $\Theta$ such that

$$0 \leq \frac{v^T A v}{v^T P v} \leq \Theta.$$

Equivalently, using (26) and noting that $v^T A v = A(v_h, v_h)$ and $v^T P v = \tilde{P}(\tilde{v}_h, \tilde{v}_h) = \| \tilde{v}_h \|^2_{P}$, it is sufficient to find $\theta$ and $\Theta$ such that

$$\theta \tilde{C} \leq \frac{\| v_h \|^2_{P}}{\| \tilde{v}_h \|^2_{P}} \leq \frac{\Theta}{2d} \quad \forall \tilde{v}_h \in \hat{V}_{h,0}.$$ 

with $v_h = \tilde{v}_h \circ G^{-1}$. Using Proposition 5, we can conclude that the previous inequalities hold with $\theta := \frac{1}{2dQ_2}$ and $\Theta := \frac{2d}{Q_1}$. \qed

4.3 Preconditioner implementation by Fast Diagonalization

The application of the preconditioner is a solution of a Sylvester-like equation: given \( r \) find \( s \) such that

\[ Ps = r. \tag{27} \]

Following [24], to solve (27), we use the Fast Diagonalization (FD) method (see [9] and [22] for further details). It is a direct method that, at the first step, computes the eigendecomposition of the pencils \((\tilde{M}_i, \tilde{J}_i)\) for \( i = 1, \ldots, d \) and of \((\hat{M}_i, \hat{K}_i)\), i.e.

\[
\tilde{J}_i U_i = \tilde{M}_i U_i \Lambda_i, \quad \hat{K}_i U_i = \hat{M}_i U_i \Lambda_i
\]

where \( \Lambda_i \) and \( \Lambda_s \) are diagonal eigenvalue matrices while the columns of \( U_i \) and \( U_t \) contain the corresponding generalized eigenvectors and they are such that

\[
\tilde{M}_i = U_i^{-T} U_i^{-1}, \quad \hat{J}_i = U_i^{-T} \Lambda_i U_i^{-1}, \quad \hat{M}_i = U_i^{-T} U_i^{-1}, \quad \hat{K}_i = U_i^{-T} \Lambda_i U_i^{-1}.
\]

Let \( U_s := U_d \otimes \cdots \otimes U_1 \) and \( \Lambda_s := \sum_{i=1}^d I_n^{-1} \otimes \Lambda_i \otimes I_{n_s}^{-1} \), where \( I_n \in \mathbb{R}^{m \times m} \) denotes the identity matrix of size \( m \). Then, \( P \) can be factorized as

\[
P = (U_t \otimes U_s)^{-T} (\Lambda_t \otimes I_n + I_n \otimes \Lambda_s)(U_t \otimes U_s)^{-1},
\]

where we have used (17), (18) and (19). Therefore, the solution of (27) can be obtained by the following algorithm:

**Algorithm 1 FD method**

1: Compute the generalized eigendecompositions (28).
2: Compute \( \tilde{\omega} = (U_t \otimes U_s)^T s \).
3: Compute \( \tilde{q} = (\Lambda_t \otimes I_n + I_n \otimes \Lambda_s)^{-1} \tilde{s} \).
4: Compute \( r = (U_t \otimes U_s) \tilde{q} \).

4.4 Inclusion of the geometry information in the preconditioner

The spectral estimates in Section 4.2.1 show the dependence on \( G \) (see the proof of Theorem 2): the geometry parametrization affects the performance of our preconditioner (25), as it is confirmed by the numerical tests in Section 5. In this section we present a strategy to partially incorporate \( G \) in the preconditioner, without increasing its computational cost. The same idea has been used in [23] for the Stokes problem. A complete analysis of this strategy will be addressed in a forthcoming work.

We split the bilinear form \( \mathcal{A}(\cdot, \cdot) \) as

\[
\mathcal{A}(v_h, w_h) = \mathcal{K}_t(v_h, w_h) + \mathcal{K}_s(v_h, w_h) - \mathcal{O}(v_h, w_h) \quad \forall v_h, w_h \in V_{h,0}
\]

where

\[
\mathcal{K}_t(v_h, w_h) := \int_{\Omega} \int_0^T \partial_t v_h \partial_t w_h \, d\Omega \, dt, \quad \mathcal{K}_s(v_h, w_h) := \int_{\Omega} \int_0^T \Delta v_h \Delta w_h \, d\Omega \, dt,
\]

\[
\mathcal{O}(v_h, w_h) := \int_{\Omega} \int_0^T (\partial_t v_h \Delta w_h + \partial_t w_h \Delta v_h) \, d\Omega \, dt.
\]

Using that \( v_h := \tilde{v}_h \circ G^{-1}, \ w_h := \tilde{w}_h \circ G^{-1} \) and

\[
\frac{\partial^2 v_h}{\partial x_i^2} = \sum_{j,k=1}^d \frac{\partial^2 \tilde{v}_h}{\partial \eta_j \partial \eta_k} [J_F^{-1}]_{kj} [J_F^{-1}]_{ji} + \sum_{j=1}^d \frac{\partial \tilde{v}_h}{\partial \eta_j} \frac{\partial G^{-1}}{\partial \eta_j} \frac{\partial [J_F^{-1}]}{\partial \eta_i},
\]

we can rewrite \( \mathcal{K}_t \) and \( \mathcal{K}_s \) as

\[
\mathcal{K}_t(v_h, w_h) = \int_{\tilde{\Omega}} \int c_r \partial_r \tilde{v}_h \partial_r \tilde{w}_h \, d\tilde{\Omega} \, dr, \quad \mathcal{K}_s(v_h, w_h) = \mathcal{K}_{s,1}(\tilde{v}_h, \tilde{w}_h) + \mathcal{K}_{s,2}(\tilde{v}_h, \tilde{w}_h)
\]
where

\[
\begin{align*}
\mathcal{K}_{s,1}(\tilde{v}_h, \tilde{w}_h) := & \sum_{k=1}^{d} \int_{0}^{1} \int_{\Omega} c_k \frac{\partial^2 \tilde{v}_h}{\partial \eta_k^2} \frac{\partial^2 \tilde{w}_h}{\partial \eta_k^2} \, d\Omega \, dt, \\
\mathcal{K}_{s,2}(\tilde{v}_h, \tilde{w}_h) := & \sum_{r,s=1}^{d} \sum_{j,k=1}^{d} \int_{0}^{1} \int_{\Omega} g_{rsjk} \frac{\partial^2 \tilde{v}_h}{\partial \eta_k \partial \eta_j} \frac{\partial^2 \tilde{w}_h}{\partial \eta_s \partial \eta_j} \, d\Omega \, dt + \sum_{j,k=1}^{d} \int_{0}^{1} \int_{\Omega} g_{jk} \frac{\partial \tilde{v}_h}{\partial \eta_k} \frac{\partial \tilde{w}_h}{\partial \eta_j} \, d\Omega \, dt,
\end{align*}
\]

and where we have defined

\[
c_r := |\det(J_F)|^{-1}, \quad c_k := \left(\left(\|J_F^{-1}\|_F\right)^2 \right)^{1/4} |\det(J_F)|^{-1},
\]

while \(g_{rsjk}^{1}, g_{rsjk}^{2}, g_{rsjk}^{3}\) are functions that depend on the parametrization \(G\) present in \(K_1 + K_2\). In particular, we approximate \(c_k\) for \(k = 1, \ldots, d\) and \(c_r\) using to the algorithm present in \([10, 34]\) as follows:

\[
c_k(\eta, \tau) \approx \mu_1(\eta_1) \cdots \mu_{k-1}(\eta_{k-1}) \omega_k(\eta_k) \mu_{k+1}(\eta_{k+1}) \cdots \mu_d(\eta_d) \mu_k(\tau), \quad c_r(\eta, \tau) \approx \mu_1(\eta_1) \cdots \mu_d(\eta_d) \omega_1(\tau).
\]

The approximation is computed in one point per element and then it is extended by interpolation to all quadrature points. The resulting computational cost is therefore proportional to the number of elements, which for smooth splines is roughly equal to \(N_{\text{dof}}\), and independent of the degrees \(p_s\) and \(p_t\). As a consequence, the algorithm used to perform the approximation has a negligible cost in the whole iterative strategy (see [23]). This first step leads to a matrix of this form

\[
\tilde{P}^G := \tilde{K}_t^G \otimes \tilde{M}_s^G + \tilde{J}_s^G \otimes \tilde{J}_t^G,
\]

where, referring to (1) for the notation of the basis functions,

\[
\begin{align*}
\left[\tilde{K}_t^G\right]_{ij} := & \int_{0}^{1} \omega_i(\tau) \tilde{b}_{i,p_i}(\tau) \tilde{b}_{j,p_j}(\tau) \, d\tau, \quad \left[\tilde{M}_s^G\right]_{ij} := \int_{0}^{1} \mu_i(\tau) \tilde{b}_{i,p_i}(\tau) \tilde{b}_{j,p_j}(\tau) \, d\tau \quad i, j = 1, \ldots, n_t, \\
\tilde{J}_s := & \sum_{k=1}^{d} \tilde{M}_d^G \otimes \cdots \otimes \tilde{M}_{k-1}^G \otimes \tilde{M}_k^G \cdots \tilde{M}_1^G, \quad \tilde{M}_s := \tilde{M}_d^G \otimes \cdots \otimes \tilde{M}_1^G,
\end{align*}
\]

with for \(i, j = 1, \ldots, n_s, k = 1, \ldots, d,\)

\[
\begin{align*}
\left[\tilde{J}_k^G\right]_{ij} := & \int_{0}^{1} \omega_i(\eta_k) \tilde{b}_{i,p_i}(\eta_k) \tilde{b}_{j,p_j}(\eta_k) \, d\eta_k, \quad \left[\tilde{M}_k^G\right]_{ij} := \int_{0}^{1} \mu_i(\eta_k) \tilde{b}_{i,p_i}(\eta_k) \tilde{b}_{j,p_j}(\eta_k) \, d\eta_k.
\end{align*}
\]

The matrix \(\tilde{P}^G\) maintains the Kronecker structure of (25) and Algorithm 1 can still be used to compute its application.

Finally, as in [23], we apply a diagonal scaling and we define the preconditioner as \(P^G := D^{1/2} \tilde{P}^G D^{1/2}\) where \(D\) is a diagonal matrix whose diagonal entries are \(D_{ii} := |A|_{ii}/|\tilde{P}^G|_{ii}\).

### 4.5 Computational cost of the linear solver

The computational cost associated with our preconditioning strategies consists of two parts: setup cost and application cost.

The setup cost of both \(P\) and \(P^G\) includes the eigendecomposition of the pencils \((\tilde{J}_t, \tilde{M}_t)\) and \((\tilde{K}_t, \tilde{M}_t)\) or \((\tilde{J}_t^G, \tilde{M}_t^G)\) and \((\tilde{K}_t^G, \tilde{M}_t^G)\), respectively, that is, Step 1 of Algorithm 1. If we assume for simplicity that \(\tilde{J}_t, \tilde{M}_t, \tilde{J}_t^G, \tilde{M}_t^G\) for \(i = 1, \ldots, d\) have size \(n_s \times n_s\) and that \(\tilde{K}_t, \tilde{M}_t, \tilde{K}_t^G\) and \(\tilde{M}_t^G\) have size \(n_t \times n_t\), the cost of the eigendecomposition is \(O(dn_s^3 + n_t^3)\) FLOPs, that is, optimal for \(d = 2\) and negligible for \(d = 3\). For \(P^G\), we also have to include in the setup cost the creation of the diagonal matrix \(D\), which
is negligible, and the construction of the \(2(d + 1)\) univariate coefficients \(\mu_1, \ldots, \mu_d, \mu_t\) and \(\omega_1, \ldots, \omega_d, \omega_t\), that are used to incorporate some geometry information into the preconditioner. As explained in Section 4.4, this has a cost which is \(O(N_{\text{dof}})\) FLOPs.

The application of \(P\) and \(\bar{P}_{\text{G}}\) is performed by Algorithm 1, Steps 2-4. Step 3 has an optimal cost, as it requires \(O(N_{\text{dof}})\) FLOPs. Step 2 and Step 4 need a total of \(4(dn_s^d+1)n_t + n_t^2n_d^2) = 4N_{\text{dof}}(dn_s + n_t)\) FLOPs. Therefore, the total cost of Algorithm 1 is \(4N_{\text{dof}}(dn_s + n_t) + O(N_{\text{dof}})\) FLOPs. The non-optimal dominant cost is given by the dense matrix-matrix products of Step 2 and Step 4, which, however, are usually implemented on modern computers in a high-efficient way, as they are BLAS level 3 operations. In our numerical tests, the overall serial computation time grows almost as \(O(N_{\text{dof}})\) up to the largest problem considered, as we will show in Section 5.

Clearly, the computation cost of each iteration of the CG solver depends on both the preconditioner application and the residual computation. For the sake of completeness, we also discuss the cost of the residual computation, which consists in the multiplication between \(A\) and a vector. Note that this multiplication can be computed by exploiting the structure (22) and the formula (20). In this case, we do not need to compute and store the whole matrix \(A\), but only its factors \(K_t, W_t, M_t, J_s, and M_s\). With this matrix-free approach, the computational cost of a single matrix-vector product is \(~6(2p+1)^2N_{\text{dof}}, if p = p_s \approx p_t\). Even if this cost is lower than what one would get by using \(A\) explicitly, the comparison with the preconditioner’s cost shows that the residual computation easily turns out to be the dominant cost of the iterative solver (see Table 3 in Section 5). This issue was already recognized in [24, 23].

We emphasize that it is possible, though beyond the scope of this paper, to take the matrix-free paradigm one step further by using the approach developed in [25]. Using this approach, where even the factors of \(A\) as in (22) are not needed, would significantly improve the overall iterative solver in terms of memory and computational cost (both for the setup and for the matrix-vector computations).

5 Numerical benchmarks

In this Section, first, we show experiments in a 2D domain that confirm the convergence behaviour (16) of the least-squares approximation method defined in Section 3.2, then we present some numerical results regarding the performance of our preconditioner.

The tests are performed with Matlab R2016a and GeoPDEs toolbox [33], on a Intel Core i7-5820K processor, running at 3.30 GHz, with 64 GB of RAM. We force the execution to be sequential and to use only a single computational thread.

In Algorithm 1, the eigendecomposition of Step 1 is done by \texttt{eig} Matlab function, while the multiplications of Kronecker matrices, appearing in Step 2 and 4, are performed by Tensorlab toolbox [28]. We fix the tolerance of CG equal to \(10^{-8}\) and the initial guess equal to the null vector in all tests.

We set \(h_s = h_t =: h\), and we denote the number of elements in each parametric direction by \(n_{\text{el}}\).

Orders of convergence. We set \(T = 1\) and we consider a 2D spatial domain: the quarter of annulus with internal radius equal to 1 and external radius equal to 2 (see Figure 1a). The initial and Dirichlet boundary conditions are fixed such that the exact solution is \(u = -(x^2 + y^2 - 1)(x^2 + y^2 - 4)xy^2 \sin(\pi t)\).

Figure 2a shows the \(||·||_{v_n}\) relative errors with splines of degree \(p_s = p_t\) from 2 to 6: the rate of convergence of \(O(h^{p_n-1})\) confirms the results of Theorem 1. As predicted by the theory, if we increase the degree of spatial B-splines and we set \(p_s = p_t + 1\), we can gain an order of convergence. Indeed, Figure 2b shows that in this case the \(||·||_{v_n}\) relative errors have order \(p_t\).

Even if theoretical results do not cover this case, we also analyze in Figures 2c and 2d the error behaviour for \(p_s = p_t\) in \(L^2(\Omega \times [0, T])\) and \(H^1(\Omega \times [0, T])\) norms, respectively. While the \(H^1\) errors are optimal for every \(p_t\) considered, i.e. they are of order \(p_t\) for \(p_t \geq 2\), the orders of convergence in \(L^2\) norm are optimal and thus equal to \(p_s + 1\), only for \(p_s \geq 3\). The suboptimal behaviour of the error in \(L^2\) norm for \(p_s = p_t = 2\) is in fact consistent with the Aubin-Nitsche type estimate and with the a-priori error estimates for fourth-order PDEs (see in particular the classical [30, Theorem 3.7]).

Performance of the preconditioner To assess the performance of our preconditioning strategy, we set \(T = 1\) and we focus on two 3D spatial domains \(\Omega \subset \mathbb{R}^3\), represented in Figure 1b and Figure 1c: the
(a) Quarter of annulus.

(b) Cube.

(c) Rotated quarter of annulus.

Figure 1: Computational domains.
The setup time of the preconditioner. The symbol "*" is used when the construction of the matrix.

Incomplete Cholesky with zero fill-in (IC(0)) factorization of

As discussed in the previous section, the matrix-vector products of CG are computed in a matrix-free way using its factors as in (22). Matrix \( \hat{A} \) is still assembled in order to use the IC(0) preconditioner. In any case, the assembly times are never included in the reported times.

We first consider the domain \( \Omega = [0,1]^3 \) (Figure 1b). Note that in this case we have that \( |P|_{ij} = \hat{P}(\hat{B}_{ij,p}, \hat{B}_{ij,p}) = \mathcal{P}(B_{ij,p}, B_{ij,p}) \). We set homogeneous Dirichlet and zero initial boundary conditions and we fix \( f \) such that the exact solution is \( u = \sin(\pi x) \sin(\pi y) \sin(\pi z) \sin(t) \).

Table 1 shows the performance of \( P \) and IC(0) preconditioners in the case \( p = p_s \). The number of iterations obtained with \( P \) are stable w.r.t. \( p_k \) and \( n_{el} \). Even if the number of iterations of our strategy might be larger than that of IC(0), the overall computation time is significantly lower, up to two orders of magnitude for the problems considered. This is due to the higher setup and application cost of the IC(0) preconditioner.

Then we consider as computational domain \( \Omega \) a quarter of annulus with center in the origin, internal radius 1 and external radius 2, rotated along the axis \( y = -1 \) by \( \pi/2 \) (see Figure 1c). Boundary data and forcing function are set such that the exact solution is \( u = -(x^2 + y^2 - 1)(x^2 + y^2 - 4)xy^2 \sin(z) \sin(t) \).

Table 2 shows the results of CG coupled with \( P \), \( P^G \) or IC(0) preconditioner. From the spectral estimates of Theorem 2, we know that the geometry parametrization \( G \), which in this case is not trivial, plays a key role in the performance of \( P \). This is confirmed by the results of Table 2: the number of iterations is higher than the ones obtained in the cube domain, where \( G \) is the identity map (see Table 1). However, the inclusion of some geometry information, and thus the use of \( P^G \) as a preconditioner, improves the performances, as we can see from the middle table of Table 2. Moreover, we show that IC(0) is not competitive neither with \( P \) nor with \( P^G \), in terms of computation time.

For the last domain, we analyze the percentage of computation time of a \( P^G \) application with respect to the overall CG time. The results, reported in Table 3, show that the time spent in the preconditioner...
application takes only a little amount of the overall solving time. The dominant cost, in this implementation is due to the matrix-vector products of the residual computation, that is the other main operation performed in a CG cycle.

Since we are primarily interested in the preconditioner performance, in Figure 3 we report in a log-log scale the computation times required for the setup and for a single application of $P_G$ versus the number of degrees-of-freedom. We see that the setup time is clearly asymptotically proportional to $N_{dof}$, as expected. Remarkably, the single application time grows slower than the expected theoretical cost $O(N_{dof}^5/4)$; indeed, it grows almost as the optimal rate $O(N_{dof})$, even for the largest problems tested. As already mentioned, this is likely due to the high efficiency of the BLAS level 3 routines that perform the computational core of the preconditioner’s application.

6 Conclusions

In this paper we have proposed and studied a least-squares formulation for the heat equation. This formulation allows us to design an innovative preconditioner in the framework of isogeometric analysis. The preconditioner $P$ that we have presented can be applied efficiently thanks to its structure: its matrix representation is a suitable sum of Kronecker products, leading to a Sylvester-like problem. The preconditioner $P$ is robust with respect to the spline degree and meshsize and its variant, denoted $P_G$, has a good performance also when the geometry parametrization $G$ of the patch is not trivial.

Numerical results showed a comparison with a preconditioner based on an Incomplete Cholesky factorization of the system matrix $A$: the solving times are significantly lower for our preconditioners, indicating that it is a promising approach.

Our preconditioning strategy can be coupled with a matrix-free approach (see [25]), and this is expected to significantly improve the performance of the overall method. We also remark that the preconditioner we propose is well-suited for parallelization. Even though in this paper we do not consider parallel implementation, this is a promising research direction for the future.

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### Table 2: Rotated quarter domain with $p_t = p_s$. Performance of $P + CG$ (upper table), $P^G + CG$ (middle table) and of IC(0)+CG (lower table).

| $n_{sub}$ | $p_t = 2$ | $p_t = 3$ | $p_t = 4$ | $p_t = 5$ |
|-----------|-----------|-----------|-----------|-----------|
|           | Iterations / Time | Iterations / Time | Iterations / Time | Iterations / Time |
| 8         | 107 / 0.21 | 107 / 0.48 | 114 / 1.17 | 123 / 2.73 |
| 16        | 126 / 2.56 | 128 / 6.90 | 133 / 17.04 | 135 / 35.177 |
| 32        | 142 / 52.77 | 143 / 132.24 | 148 / 292.53 | 151 / 572.84 |
| 64        | 153 / 1056.21 | 155 / 2415.23 | 156 / 4956.68 | 159 / 9906.33 |
| 128       | 164 / 22106.01 | * | 166 / 47539.02 | * |

### Table 3: Rotated quarter domain with $p_t = p_s$. Percentage of computation time of the preconditioner $P^G$ application in the overall CG cycle.

| $n_{sub}$ | $p_t = 2$ | $p_t = 3$ | $p_t = 4$ | $p_t = 5$ |
|-----------|-----------|-----------|-----------|-----------|
|           | $P^G$    | $P^G$    | $P^G$    | $P^G$    |
| 8         | 35.86%   | 20.66%   | 10.85%   | 7.05%    |
| 16        | 17.90%   | 8.10%   | 3.95%   | 2.28%    |
| 32        | 14.25%   | 7.35%   | 4.05%   | 2.49%    |
| 64        | 17.28%   | 8.75%   | 4.67%   | 2.52%    |
| 128       | 23.98%   | 12.21%  | *       | *        |
Figure 3: Rotated quarter domain with $p_t = p_s$. Setup times and single application times of $P^G$. 
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A Appendix

A.1 Regularity of the solution

Thanks to Assumptions 3-4, we have that $F : \hat{\Omega} \to \Omega$ fulfills $F \in C^{1,1}$ on the closure of $\hat{\Omega}$ and $F^{-1} \in C^{1,1}(\Omega)$. Under these conditions, the following regularity results hold.

Lemma 5. If $f \in L^2(\Omega)$, there exists a unique weak solution $u \in H^2(\Omega)$ to the Poisson problem

$$
\left\{
\begin{array}{ll}
-\Delta u = f & \text{in } \Omega, \\
u = 0 & \text{on } \partial \Omega.
\end{array}
\right.
$$

Moreover, there exists a constant $C$ depending only on $\|F\|_{L^2,\infty(\Omega)}$ such that

$$
\|u\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\Omega)}.
$$

Proof. We recall that $u$ is a weak solution of (29) if $u \in H^1_0(\Omega)$ and if $\int_{\Omega} \nabla u \cdot \nabla v \, d\Omega = \int_{\Omega} f v \, d\Omega \ \forall v \in H^1_0(\Omega)$. We have that $u \in H^1_0(\Omega)$ is a weak solution of (29) if and only if $w := u \circ F \in H^1_0(\hat{\Omega})$ is a weak solution of

$$
\left\{
\begin{array}{ll}
-\nabla \cdot (R \nabla w) = g & \text{in } \hat{\Omega}, \\
w = 0 & \text{on } \partial \hat{\Omega},
\end{array}
\right.
$$

where $g := |\det(J_F)|f \circ F$ and $R := J_F^{-1}J_F^{-T}|\det(J_F)|$. Thanks to the regularity assumptions on $F$ and $F^{-1}$ recalled above, we have that the entries of the matrix $R$ are Lipschitz continuous and we can apply [13, Theorem 3.2.1.2] to conclude that there exist a unique solution $w \in H^2(\hat{\Omega})$ of problem (31). Thanks to [19, Lemma 11.1] we also have

$$
\|w\|^2_{H^2(\hat{\Omega})} \leq c_1 \left(\|\nabla \cdot (R \nabla w)\|^2_{L^2(\hat{\Omega})} + \|w\|^2_{L^2(\hat{\Omega})}\right) \leq c_2 \|\nabla \cdot (R \nabla w)\|^2_{L^2(\hat{\Omega})} = c_2\|g\|^2_{L^2(\hat{\Omega})},
$$

where $c_1$ and $c_2$ are constants depending only on $F$ and $F^{-1}$. Finally, we conclude

$$
\|u\|_{H^2(\Omega)} \leq C_1\|w\|_{H^2(\hat{\Omega})} \leq C_2\|g\|_{L^2(\hat{\Omega})} \leq C\|f\|_{L^2(\Omega)},
$$

where the constants $C_1, C_2$ and $C$ depend only on $\|F\|_{L^2,\infty(\Omega)}$, $F$ and $F^{-1}$. □

Theorem 3. Let $f \in L^2(\Omega \times (0,T))$. Then there exists a unique weak solution (as defined in [11, Chapter 7]) $u \in \left(H^2(\Omega) \cap L^2(0,T)\right) \cap \left(L^2(\Omega) \cap H^1(0,T)\right)$ of (5). We also have

$$
\|u\|_{H^2(\Omega) \cap L^2(0,T)} + \|u\|_{L^2(\Omega) \cap H^1(0,T)} \leq C\|f\|_{L^2(\Omega \times (0,T))},
$$

where $C$ is a constant depending only on $\|F\|_{L^2,\infty(\Omega)}$, $F$ and $F^{-1}$.

Proof. Following the same arguments of step 1 and step 2 of the proof of [11, Theorem 5], we conclude that $u \in \left(H^1_0(\Omega) \cap L^\infty(0,T)\right) \cap \left(L^2(\Omega) \cap H^1(0,T)\right)$ and that

$$
\|u\|_{H^1_0(\Omega) \cap L^\infty(0,T)} + \|u\|_{L^2(\Omega) \cap H^1(0,T)} \leq D_1\|f\|_{L^2(\Omega \times (0,T))},
$$

where $D_1$ is a constant depending only on $\|F\|_{W^{1,\infty}(\Omega)}$.

We write for a.e. $t$

$$
\int_{\Omega} \nabla u(\cdot,t) \cdot \nabla v \, d\Omega = \int_{\Omega} z(\cdot,t) \, v \, d\Omega \ \forall v \in H^1_0(\Omega),
$$

where $z := f - \partial_t u \in L^2(\Omega \times (0,T))$ and in particular $z(\cdot,t) \in L^2(\Omega)$ for a.e. $t$. Therefore, thanks to Lemma 5, we conclude that $u(\cdot,t) \in H^2(\Omega)$ for a.e. $t$ and thus $u \in H^2(\Omega) \cap L^2(0,T)$: indeed, integrating in time, (30) and (32) yield to the following estimate

$$
\|u\|^2_{H^2(\Omega) \cap L^2(0,T)} \leq C^2\|z\|^2_{L^2(\Omega \times (0,T))} \leq C^2(\|f\|^2_{L^2(\Omega \times (0,T))} + \|u\|^2_{L^2(\Omega) \cap H^1(0,T)}) \leq D^2_2\|f\|^2_{L^2(\Omega \times (0,T))},
$$

where $D^2_2 := C^2 + D^2_1$. This concludes the proof. □
A.2 A variational formulation equivalent to (8)–(9)

For sake of simplicity let us assume that \( f \in H^1(0,T; L^2(\Omega)) = L^2(\Omega) \otimes H^1(0,T) \). First of all, for \( w \in V_0 \) we write:

\[
\frac{1}{2} \int_0^T \| \partial_t w - \Delta w - f \|^2_{L^2(\Omega)} \, dt = \frac{1}{2} \int_0^T \left( \| \partial_t w \|^2_{L^2(\Omega)} + \| \Delta w + f \|^2_{L^2(\Omega)} \right) \, dt - \int_0^T \int_\Omega \partial_t w \Delta w \, d\Omega \, dt - \int_0^T \int_\Omega \partial_t w f \, d\Omega \, dt.
\]

By [6, Lemma 3.3] and since \( w = 0 \) in \( \Omega \times \{0\} \), the last terms on the right-hand side reads

\[
- \int_0^T \int_\Omega \partial_t w \Delta w \, d\Omega \, dt - \int_0^T \int_\Omega \partial_t w f \, d\Omega \, dt = \frac{1}{2} \int_\Omega |\nabla w(\mathbf{x},T)|^2 \, d\Omega - \int_\Omega f(\mathbf{x},T)w(\mathbf{x},T) \, d\Omega + \int_0^T \int_\Omega \partial_t f w \, d\Omega \, dt.
\]

At this point, let us introduce the energy \( J : H^1_0(\Omega) \times [0,T] \rightarrow \mathbb{R} \) given by

\[
J(v,t) := \int_\Omega \left( \frac{1}{2} |\nabla v(\mathbf{x})|^2 - f(\mathbf{x},t)v(\mathbf{x}) \right) \, d\Omega.
\]

Then, if \( v \in H^1_0(\Omega) \cap H_\Delta(\Omega) \) we have

\[
- \int_\Omega \partial_t f(\mathbf{x},t)v(\mathbf{x}) \, d\Omega = \partial_t J(v,t) \quad \text{and} \quad \int_\Omega (-\Delta v(\mathbf{x}) - f(\mathbf{x},t))z(\mathbf{x}) \, d\Omega = \partial_z J(v,t)[z]
\]

for all \( z \in H^1_0(\Omega) \cap H_\Delta(\Omega) \). Hence the parabolic problem turns out to be the \( L^2 \)-gradient flow for \( J \), i.e.

\[
\begin{cases}
\partial_t u = -\partial_u J(u,t) & \text{in } \Omega \times (0,T),\\
u = 0 & \text{on } \partial \Omega \times (0,T),\\
u = 0 & \text{in } \Omega \times \{0\},
\end{cases}
\]

while in terms of \( J \) and its derivatives for \( w \in V_0 \) we can write

\[
\frac{1}{2} \int_0^T \| \partial_t w - \Delta w - f \|^2_{L^2(\Omega)} \, dt = J(w(T),T) + \frac{1}{2} \int_0^T \left( \| \partial_t w \|^2_{L^2(\Omega)} + \| \partial_w J(w,t) \|^2_{L^2(\Omega)} \right) \, dt + \int_0^T \partial_t J(w,t) \, dt.
\]

In our context, \( u \in V_0 \) is a minimizer of \( \frac{1}{2} \int_0^T \| \partial_t w - \Delta w - f \|^2_{L^2(\Omega)} \, dt \) if and only if \( u \) is a curve of maximal slope, i.e. if it satisfies the energy inequality

\[
J(u(T),T) + \frac{1}{2} \int_0^T \left( \| \partial_t u \|^2_{L^2(\Omega)} + \| \partial_u J(u,t) \|^2_{L^2(\Omega)} \right) \, dt + \int_0^T \partial_t J(u,t) \, dt \leq J(u(0),0) = 0.
\]

We remark that the above inequality and the concept of curves of maximal slope extends to very general energies and functional spaces, see for instance [1, 26].

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