Technische Universität Graz

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Space-time tensor-product finite element methods for parabolic problems

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Abstract

We study space-time Galerkin–Petrov formulations for parabolic evolution problems and their relation to classical implicit time-stepping schemes. Although such schemes are stable in the usual time-stepping sense, their interpretation as space-time operator equations may lead to conditional stability, with constants depending on the relation between temporal and spatial mesh sizes. We revisit this phenomenon for the continuous Galerkin method of Aziz and Monk, which yields the Crank–Nicolson scheme in the lowest-order case, and provide a detailed space-time error analysis for solutions of both high and low regularity. In particular, the space-time framework allows us to analyze the deteriorated behaviour of classical time-stepping methods for nonsmooth initial data. By applying integration by parts in time, we derive an adjoint space-time formulation that incorporates the initial condition in a natural variational way. In the lowest-order case, this formulation leads to a Rannacher-type smoothing of the initial data. The theoretical results are complemented by numerical experiments.

1 Introduction

In this work, we are interested in the numerical solution of parabolic evolution equations using space-time methods. As a model problem, we consider the initial Dirichlet boundary value problem for the heat equation in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$, and a finite time horizon $T > 0$,

$$\begin{array}{rcll} \partial_t u(x,t) - \Delta_x u(x,t) & = & f(x,t) & \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,t) & = & 0 & \text{for } (x,t) \in \Sigma := \partial\Omega \times (0,T), \\ u(x,0) & = & u_0(x) & \text{for } x \in \Omega. \end{array} \tag{1.1}$$

A standard approach for the numerical solution of (1.1) is to first discretize the problem in space, e.g. by a finite element or finite difference method, and then solve the resulting system of ordinary differential equations by a time stepping scheme. The analysis of such schemes is well established, see, e.g., [19]. However, a classical time stepping analysis relies in most cases on point values of the solution and the right-hand side in time, called temporal collocation. Consequently, the resulting error estimates are usually formulated pointwise in time and require more regularity of the data than would be needed for estimates in natural Sobolev or Bochner spaces.

A way to overcome this limitation is to consider Galerkin–Petrov variational formulations in time. These methods can be divided into two main classes: In continuous Galerkin (cG) methods, the ansatz space consists of continuous functions in time, whereas the test space is discontinuous. Such schemes were studied, for instance, in [4, 20, 37]. In contrast, in discontinuous Galerkin (DG) methods, both ansatz and test spaces are discontinuous in time, see [14, 22, 23]. Depending on the quadrature formula used for the temporal integrals, these Galerkin–Petrov schemes are equivalent to well known time stepping methods. At the same time, their variational structure provides a framework for deriving error estimates under weaker regularity assumptions.

Instead of applying a Galerkin–Petrov formulation only to the purely temporal problem, one may also consider space-time variational formulations. These methods make use of the fact that the space-time operator equation is well-posed in suitable space-time Banach spaces. In such approaches, space and time are treated simultaneously, leading to a monolithic system rather than to a sequential time stepping procedure, see, for instance, [13, 21, 29, 30, 31, 32, 33]. This point of view is particularly attractive for adaptive methods [1, 16], time-parallel algorithms [17], and the construction of preconditioners for the resulting monolithic systems [13, 25], as well as optimal control problems subject to time dependent partial differential equations [11]. Space-time discretizations may either be built on general unstructured space-time meshes or on tensor product spaces. In both cases, stability of the discrete space-time formulation is a central issue.

A detailed analysis for cG schemes on tensor product meshes was carried out by Andreev [2]. A central observation of this analysis is that, although the corresponding time stepping scheme may be unconditionally stable in the classical sense, the associated space-time operator equation can suffer from conditional stability. More precisely, the stability constant may depend on the relation between the temporal and spatial mesh sizes, leading to a CFL-type restriction that enforces parabolic scaling. Similar conclusions were obtained in [12, 13]. Thus, the space-time perspective does not merely reproduce classical time stepping schemes, but also provides a variational framework for analyzing their deteriorated behaviour for nonsmooth data. In particular, the loss of accuracy observed for low-regularity initial conditions in classical time stepping methods [26, 36] can be understood at the level of the associated space-time operator equation, see also [3].

In this paper, we focus first on the cG scheme introduced by Aziz and Monk [4], which yields the Crank–Nicolson method in the lowest order case. We revisit the conditional stability result of [2] in a space-time framework and analyze the resulting discretization by means of an inf-sup argument. In particular, we give a detailed space-time error analysis and derive convergence rates for solutions of both high and low regularity. Furthermore, by applying integration by parts in time, we introduce an adjoint space-time formulation. This formulation incorporates the initial condition in a natural way and, in the lowest order case, leads to a scheme that can be interpreted as a Rannacher-type smoothing of the initial data [26].

The paper is structured as follows. In Section 2, we introduce the space-time variational formulation for the model problem and recall existence and uniqueness results based on the inf-sup theory. In Section 3, we collect space-time approximation estimates for functions of different regularity, which are then used in Section 4 to derive error estimates for the primal formulation. In Section 5, we apply integration by parts in time and obtain the corresponding adjoint formulation. The analysis is complemented by numerical experiments in Section 6. Finally, conclusions are given in Section 7.

2 The primal space-time variational formulation

The primal space-time variational formulation of the initial boundary value problem (1.1) is to find $u \in X$ with $u(\cdot, 0) = u_0 \in L^2(\Omega)$, such that

$$\int_0^T \int_\Omega \Big[\partial_t u(x,t)\, v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t)\Big] dx\, dt \;=\; \int_0^T \int_\Omega f(x,t)\, v(x,t)\, dx\, dt \tag{2.1}$$

is satisfied for all $v \in Y := L^2(0,T;H_0^1(\Omega))$, where $X := \{u \in Y : \partial_t u \in Y^*\}$. Related norms are given as

$$\|v\|_Y := \|\nabla_x v\|_{L^2(Q)}, \quad \|u\|_X := \sqrt{\|u\|_Y^2 + \|\partial_t u\|_{Y^*}^2} = \sqrt{\|u\|_Y^2 + \|w_u\|_Y^2},$$

where $w_u \in Y$ is the unique solution of the variational formulation

$$\int_0^T \int_\Omega \nabla_x w_u(x,t) \cdot \nabla_x v(x,t)\, dx\, dt \;=\; \int_0^T \int_\Omega \partial_t u(x,t)\, v(x,t)\, dx\, dt$$

for all $v \in Y$. For $u \in X$ and $v \in Y$ we introduce the bilinear form

$$b(u,v) \;:=\; \int_0^T \int_\Omega \Big[\partial_t u(x,t)\, v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t)\Big] dx\, dt, \tag{2.2}$$

satisfying

$$|b(u,v)| \le \sqrt{2}\, \|u\|_X \|v\|_Y \quad \text{for all } (u,v) \in X \times Y. \tag{2.3}$$

To ensure the well-posedness of the variational formulation (2.1), we assume $f \in Y^*$, and $u_0 \in L^2(\Omega)$. The latter ensures the existence of an extension $\widetilde{u}_0 \in X$ satisfying $\widetilde{u}_0(\cdot, 0) = u_0 \in L^2(\Omega)$. It remains to determine $\widetilde{u} \in X_0 := \{u \in X : u(\cdot, 0) = 0 \in L^2(\Omega)\}$ as unique solution of the variational problem

$$b(\widetilde{u} + \widetilde{u}_0, v) \;=\; \langle f, v\rangle_Q \quad \text{for all } v \in Y. \tag{2.4}$$

Unique solvability of the variational formulation (2.4) follows from the surjectivity of the bounded bilinear form $b(\cdot,\cdot)$, and from the inf-sup stability condition

$$\|u\|_X \le \sup_{0\neq v\in Y} \frac{b(u,v)}{\|v\|_Y} \quad \text{for all } u\in X_0. \tag{2.5}$$

The proof of (2.5) follows when considering the particular test function $\overline{v} := u + w_u$ for $u\in X_0\subset Y$, see [29, Theorem 2.1]. For conforming space-time finite element spaces $X_{0,h}\subset X_0$ and $Y_h\subset Y$, the Galerkin variational formulation of (2.4) is to find $\widetilde{u}_h\in X_{0,h}$ such that

$$b(\widetilde{u}_h+\widetilde{u}_0, v_h) \,=\, \langle f, v_h\rangle_Q \quad \text{for all } v_h\in Y_h. \tag{2.6}$$

Unique solvability of (2.6) and related space-time finite element error estimates follow from the discrete inf-sup stability condition

$$\|u_h\|_{X,h} \le \sup_{0\neq v_h\in Y_h} \frac{b(u_h,v_h)}{\|v_h\|_Y} \quad \text{for all } u_h\in X_{0,h}, \tag{2.7}$$

when using the discrete norm

$$\|u\|_{X,h} := \sqrt{\|u\|_Y^2 + \|w_{u,h}\|_Y^2},$$

where $w_{u,h}\in Y_h$ solves the variational formulation

$$\langle \nabla_x w_{u,h}, \nabla_x v_h\rangle_{L^2(Q)} = \langle \partial_t u, v_h\rangle_Q \quad \text{for all } v_h\in Y_h.$$

Indeed, the discrete inf-sup stability condition (2.7) follows as in the continuous case when choosing $\overline{v}_h := u_h + w_{u_h,h}\in Y_h$ for $u_h\in X_{0,h}\subset Y_h$. In [29], we have considered space-time finite element spaces $X_{0,h} = Y_h = \text{span}\{\varphi_k\}_{k=1}^M \subset X_0\subset Y$ of piecewise linear continuous basis functions φ_k which are defined with respect to an admissible locally quasi-uniform decomposition of the space-time domain Q into simplicial shape regular space-time finite elements q_ℓ of mesh size h_ℓ. However, in this paper we will consider different tensor product space-time finite element spaces $X_{0,h}\subset X_0$ and $Y_h\subset Y$ satisfying $\dim X_{0,h} = \dim Y_h$ but $X_{0,h}\not\subset Y_h$, in order to reformulate the space-time Galerkin formulation (2.6) in the spirit of more common time stepping schemes. For simplicity, in this paper we only consider lowest order space-time finite element spaces, but this approach can be extended to higher order polynomial spaces as well.

3 Space-time tensor product finite element spaces

For the spatial domain $\Omega\subset\mathbb{R}^n$ we consider an admissible and globally quasi-uniform decomposition into shape regular simplicial finite elements τ_ℓ of mesh size h_x, and the related finite element space $V_{h_x} = \text{span}\{\varphi_k\}_{k=1}^{M_x} \subset H_0^1(\Omega)$ of piecewise linear continuous basis functions φ_k. In the case of a globally quasi-uniform finite element mesh there holds the inverse inequality

$$\|\nabla_x u_h\|_{L^2(\Omega)} \,\leq\, c\, h_x^{-1}\, \|u_h\|_{L^2(\Omega)} \quad \text{for all } u_h \in V_{h_x}. \tag{3.1}$$

For $u \in L^2(\Omega)$ we introduce the L^2 projection $Q^1_{h_x} u \in V_{h_x}$ as the unique solution of the variational formulation

$$\langle Q^1_{h_x} u, v_h \rangle_{L^2(\Omega)} \,=\, \langle u, v_h \rangle_{L^2(\Omega)} \quad \text{for all } v_h \in V_{h_x},$$

for which we immediately conclude the trivial stability estimate

$$\|Q^1_{h_x} u\|_{L^2(\Omega)} \,\leq\, \|u\|_{L^2(\Omega)} \quad \text{for all } u \in L^2(\Omega). \tag{3.2}$$

When assuming $u \in H^1_0(\Omega) \cap H^s(\Omega)$ for some $s \in [1,2]$, there hold the following error estimates, e.g., [7, 28]:

$$\|u - Q^1_{h_x} u\|_{L^2(\Omega)} \;\leq\; c\, h_x^s\, |u|_{H^s(\Omega)}, \tag{3.3}$$

$$\|\nabla_x (u - Q^1_{h_x} u)\|_{L^2(\Omega)} \;\leq\; c\, h_x^{s-1}\, |u|_{H^s(\Omega)}. \tag{3.4}$$

Using (3.3) and (3.4), and a space interpolation argument for some $\tau \in [0,1]$, we conclude the error estimate

$$\|u - Q^1_{h_x} u\|_{H^\tau(\Omega)} \,\leq\, c\, h_x^{s-\tau}\, |u|_{H^s(\Omega)}. \tag{3.5}$$

Moreover, e.g., [6], $Q^1_{h_x} : H^1_0(\Omega) \subset L^2(\Omega) \to V_{h_x} \subset H^1_0(\Omega)$ is stable in $H^1_0(\Omega)$, i.e.,

$$\|\nabla_x Q^1_{h_x} u\|_{L^2(\Omega)} \,\leq\, c_Q\, \|\nabla_x u\|_{L^2(\Omega)} \quad \text{for all } u \in H^1_0(\Omega). \tag{3.6}$$

In addition to the L^2 projection $Q^1_{h_x} u$ we introduce, for $u \in H^1_0(\Omega)$, the H^1_0 projection $P^1_{h_x} u \in V_{h_x}$ as the unique solution of the variational formulation

$$\langle \nabla_x P^1_{h_x} u, \nabla_x v_h \rangle_{L^2(\Omega)} \,=\, \langle \nabla_x u, \nabla_x v_h \rangle_{L^2(\Omega)} \quad \text{for all } v_h \in V_{h_x}, \tag{3.7}$$

where we conclude the stability estimate

$$\|\nabla_x P^1_{h_x} u\|_{L^2(\Omega)} \,\leq\, \|\nabla_x u\|_{L^2(\Omega)} \quad \text{for all } u \in H^1_0(\Omega), \tag{3.8}$$

and the error estimates

$$\|\nabla_x (u - P^1_{h_x} u)\|_{L^2(\Omega)} \;\leq\; c\, h_x^{s-1}\, |u|_{H^s(\Omega)}, \tag{3.9}$$

$$\|u - P^1_{h_x} u\|_{L^2(\Omega)} \;\leq\; c\, h_x^s\, |u|_{H^s(\Omega)}, \tag{3.10}$$

when assuming $u \in H^1_0(\Omega) \cap H^s(\Omega)$ for some $s \in [1,2]$.

For the time interval $(0,T)$ we consider a uniform decomposition into N_t finite elements (t_{i-1}, t_i) of mesh size $h_t = T/N_t$, and nodes $t_i = i h_t$ for $i = 0, \ldots, N_t$. With respect to this temporal mesh we introduce the space $S^1_{h_t}(0,T) = \text{span}\{\psi^1_i\}_{i=0}^{N_t}$ of piecewise linear and continuous basis functions ψ_i^1. For continuous $u \in H^\sigma(0,T)$, $\sigma > \frac{1}{2}$, we define the nodal interpolation

$$(I_{h_t}^1 u)(t) = \sum_{i=0}^{N_t} u(t_i)\psi_i^1(t)\,, \tag{3.11}$$

for which we have the error estimate

$$\|u - I_{h_t}^1 u\|_{L^2(0,T)} \leq c\, h_t^\sigma\, |u|_{H^\sigma(0,T)}, \tag{3.12}$$

when assuming $u \in H^\sigma(0,T)$ for some $\sigma \in (1/2, 2]$. Note that the constant degenerates as $\sigma \to 1/2$. Finally, $W_{h_t}^0 = \operatorname{span}\{\psi_i^0\}_{i=1}^{N_t} \subset L^2(0,T)$ is the space of piecewise constant basis functions ψ_i^0, for which the temporal L^2 projection $Q_{h_t}^0 u \in W_{h_t}^0$ is defined as the unique solution of the variational formulation

$$\langle Q_{h_t}^0 u, v_h\rangle_{L^2(0,T)} = \langle u, v_h\rangle_{L^2(0,T)} \quad \text{for all } v_h \in W_{h_t}^0, \tag{3.13}$$

satisfying the error estimate

$$\|u - Q_{h_t}^0 u\|_{L^2(0,T)} \;\leq\; c\, h_t^\sigma\, |u|_{H^\sigma(0,T)}, \tag{3.14}$$

when assuming $u \in H^\sigma(0,T)$ for some $\sigma \in [0,1]$. For $t \in (t_{i-1}, t_i)$ we finally compute

$$\partial_t I_{h_t}^1 u(t) = \frac{1}{h_t}\,(u(t_i) - u(t_{i-1})) = \frac{1}{h_t}\int_{t_{i-1}}^{t_i} \partial_t u(t)\, dt = Q_{h_t}^0 \partial_t u(t)\,.$$

Now we are in a position to state some approximation error estimates in space-time tensor product finite element spaces:

Lemma 3.1 *Let $u \in L^2(0,T; H_0^1(\Omega) \cap H^s(\Omega)) \cap H^\sigma(0,T; H_0^1(\Omega))$ for some $s \in [1,2]$ and $\sigma \in (1/2, 2]$. Then there holds the error estimate*

$$\|\nabla_x(u - Q_{h_x}^1 I_{h_t}^1 u)\|_{L^2(Q)} \;\leq\; c_1\, h_x^{s-1}\, |u|_{L^2(0,T;H^s(\Omega))} + c_2\, h_t^\sigma\, |u|_{H^\sigma(0,T;H_0^1(\Omega))}. \tag{3.15}$$

If $u \in L^2(0,T; H_0^1(\Omega) \cap H^s(\Omega)) \cap H^\sigma(0,T; L^2(\Omega))$ is satisfied for some $s \in [1,2]$ and $\sigma \in (1/2, 2]$, then there holds the error estimate

$$\|\nabla_x(u - Q_{h_x}^1 I_{h_t}^1 u)\|_{L^2(Q)} \;\leq\; c_1\, h_x^{s-1}\, |u|_{L^2(0,T;H^s(\Omega))} + c_2\, h_x^{-1}\, h_t^\sigma\, |u|_{H^\sigma(0,T;L^2(\Omega))}. \tag{3.16}$$

Proof. By the triangle inequality, we first have

$$\|\nabla_x(u - Q_{h_x}^1 I_{h_t}^1 u)\|_{L^2(Q)} \;\leq\; \|\nabla_x(u - Q_{h_x}^1 u)\|_{L^2(Q)} + \|\nabla_x Q_{h_x}^1(u - I_{h_t}^1 u)\|_{L^2(Q)}. \tag{3.17}$$

For the first part we can use the error estimate (3.4) for $s \in [1,2]$ to conclude

$$\begin{aligned}
\|\nabla_x(u - Q_{h_x}^1 u)\|_{L^2(Q)}^2 \;&=\; \int_0^T \|\nabla_x(u(t) - Q_{h_x}^1 u(t))\|_{L^2(\Omega)}^2\, dt \\
&\leq\; c\, h_x^{2(s-1)} \int_0^T |u(t)|_{H^s(\Omega)}^2\, dt,
\end{aligned}$$

i.e.,
$$\|\nabla_x(u - Q^1_{h_x}u)\|_{L^2(Q)} \,\leq\, c\, h_x^{s-1}\, |u|_{L^2(0,T;H^s(\Omega))}.$$
To bound the second term in (3.17), we first use the stability estimate (3.6) and the interpolation error estimate (3.12) to obtain
$$\begin{aligned}
&\|\nabla_x Q^1_{h_x}(u - I^1_{h_t}u)\|^2_{L^2(Q)} \,=\, \int_0^T \|\nabla_x Q^1_{h_x}(u(t) - I^1_{h_t}u(t))\|^2_{L^2(\Omega)}\, dt \\
&\leq\, c_Q^2 \int_0^T \|\nabla_x(u(t) - I^1_{h_t}u(t))\|^2_{L^2(\Omega)}\, dt \,=\, c_Q^2 \int_\Omega \|(I - I^1_{h_t})\nabla_x u(x)\|^2_{L^2(0,T)}\, dx \\
&\leq\, c\, h_t^{2\sigma} \int_\Omega \|\nabla_x u\|^2_{H^\sigma(0,T)}\, dx \,=\, c\, h_t^{2\sigma}\, \|\nabla_x u\|^2_{H^\sigma(0,T;L^2(\Omega))},
\end{aligned}$$
i.e.,
$$\|\nabla_x Q^1_{h_x}(u - I^1_{h_t}u)\|_{L^2(Q)} \,\leq\, c\, h_t^{\sigma}\, \|u\|_{H^\sigma(0,T;H^1_0(\Omega))},$$
and (3.15) follows.

However, when using the inverse inequality (3.1) in space first, the stability estimate (3.2), and the temporal interpolation error estimate (3.12), we obtain
$$\begin{aligned}
\|\nabla_x Q^1_{h_x}(u - I^1_{h_t}u)\|^2_{L^2(Q)} \;&=\; \int_0^T \|\nabla_x Q^1_{h_x}(u - I^1_{h_t}u)\|^2_{L^2(\Omega)}\, dt \\
&\leq\; c\, h_x^{-2} \int_0^T \|Q^1_{h_x}(u(t) - I^1_{h_t}u(t))\|^2_{L^2(\Omega)}\, dt \\
&\leq\; c\, h_x^{-2} \int_0^T \|u(t) - I^1_{h_t}u(t)\|^2_{L^2(\Omega)}\, dt \\
&=\; c\, h_x^{-2} \int_\Omega \|u(x) - I^1_{h_t}u(x)\|^2_{L^2(0,T)}\, dx \\
&\leq\; c\, h_x^{-2}\, h_t^{2\sigma} \int_\Omega |u(x)|^2_{H^\sigma(0,T)}\, dx,
\end{aligned}$$
i.e.,
$$\|\nabla_x Q^1_{h_x}(u - I^1_{h_t}u)\|_{L^2(Q)} \,\leq\, c\, h_x^{-1}\, h_t^{\sigma}\, \|u\|_{H^\sigma(0,T;L^2(\Omega))},$$
and this gives (3.16). ■

When the nodal piecewise linear interpolation $I^1_{h_t}$ in time is replaced by the temporal piecewise constant L^2 projection $Q^0_{h_t}$, the statement of Lemma 3.1 can be reformulated as follows, where the proof can be adapted accordingly.

Lemma 3.2 *Let $u \in L^2(0,T;H^1_0(\Omega) \cap H^s(\Omega)) \cap H^\sigma(0,T;H^1_0(\Omega))$ for some $s \in [1,2]$ and $\sigma \in [0,1]$. Then there holds the error estimate*
$$\|\nabla_x(u - Q^1_{h_x}Q^0_{h_t}u)\|_{L^2(Q)} \,\leq\, c_1\, h_x^{s-1}\, |u|_{L^2(0,T;H^s(\Omega))} + c_2\, h_t^{\sigma}\, |u|_{H^\sigma(0,T;H^1_0(\Omega))}. \tag{3.18}$$
If $u \in L^2(0,T;H^1_0(\Omega) \cap H^s(\Omega)) \cap H^\sigma(0,T;L^2(\Omega))$ is satisfied for some $s \in [1,2]$ and $\sigma \in [0,1]$, then there holds the error estimate
$$\|\nabla_x(u - Q^1_{h_x}Q^0_{h_t}u)\|_{L^2(Q)} \,\leq\, c_1\, h_x^{s-1}\, |u|_{L^2(0,T;H^s(\Omega))} + c_2\, h_x^{-1}\, h_t^{\sigma}\, |u|_{H^\sigma(0,T;L^2(\Omega))}. \tag{3.19}$$

It remains to state an approximation result for $Q^1_{h_x} I^1_{h_t}$ in Y^*:

Lemma 3.3 *For $u \in X \cap H^\varrho(0,T;H^{-1}(\Omega))$, let $\partial_t u \in L^2(0,T;H^{-\tau}(\Omega))$ be satisfied for some $\tau \in [0,1]$, and $\varrho \in [1,2]$. Then there holds the error estimate*

$$\|\partial_t(u - Q^1_{h_x} I^1_{h_t} u)\|_{Y^*} \, \leq \, c_1 \, h_x^{1-\tau} \, \|\partial_t u\|_{L^2(0,T;H^{-\tau}(\Omega))} \, + \, c_2 \, h_t^{\varrho-1} \, \|u\|_{H^\varrho(0,T;H^{-1}(\Omega))}. \tag{3.20}$$

Proof. For any $v \in Y = L^2(0,T;H^1_0(\Omega))$, we first consider

$$\begin{aligned} \langle \partial_t(u - Q^1_{h_x} I^1_{h_t} u), v\rangle_Q &= \langle \partial_t u - Q^1_{h_x} \partial_t u, v\rangle_Q + \langle Q^1_{h_x}(\partial_t u - \partial_t I^1_{h_t} u), v\rangle_Q \\ &= \langle \partial_t u, (I - Q^1_{h_x}) v\rangle_Q + \langle \partial_t u - \partial_t I^1_{h_t} u, Q^1_{h_x} v\rangle_Q \, . \end{aligned}$$

For the first part, we obtain, using duality and the error estimate (3.5) for some $\tau \in (0,1]$,

$$\begin{aligned} \langle \partial_t u, (I - Q^1_{h_x}) v\rangle_Q &\leq \|\partial_t u\|_{L^2(0,T;H^{-\tau}(\Omega))} \, \|(I - Q^1_{h_x}) v\|_{L^2(0,T;H^\tau_0(\Omega))} \\ &\leq c \, h_x^{1-\tau} \, \|\partial_t u\|_{L^2(0,T;H^{-\tau}(\Omega))} \, \|v\|_{L^2(0,T;H^1_0(\Omega))} \, . \end{aligned}$$

For the remaining term we conclude, using $\partial_t I^1_{h_t} u = Q^0_{h_t} \partial_t u$, duality, the stability estimate (3.6), and the error estimate (3.14),

$$\begin{aligned} \langle \partial_t u - \partial_t I^1_{h_t} u, Q^1_{h_x} v\rangle_Q &= \langle (I - Q^0_{h_t}) \partial_t u, Q^1_{h_x} v\rangle_Q \\ &\leq \|(I - Q^0_{h_t}) \partial_t u\|_{L^2(0,T;H^{-1}(\Omega))} \, \|Q^1_{h_x} v\|_{L^2(0,T;H^1_0(\Omega))} \\ &\leq c \, h_t^{\varrho-1} \, \|u\|_{H^\varrho(0,T;H^{-1}(\Omega))} \, \|v\|_{L^2(0,T;H^1_0(\Omega))}, \end{aligned}$$

and the assertion follows from the norm definition of $\|\partial_t(u - Q^1_{h_x} I^1_{h_t} u)\|_{Y^*}$ by duality. ∎

4 The primal space-time finite element method

For a space-time tensor product finite element formulation of (2.6) we consider the ansatz space $X_{0,h} := W^1_{h_t} \otimes V_{h_x} \subset X_0$ with $W^1_{h_t} = S^1_h(0,T) \cap H^1_{0,}(0,T) = \text{span}\{\psi^1_i\}_{i=1}^{N_t}$, and the test space $Y_h := W^0_{h_t} \otimes V_{h_x} \subset Y$. By construction we have $\dim X_{0,h} = \dim Y_h = N_t \, M_x$, but $X_{0,h} \not\subset Y_h$. In this case, unique solvability of (2.6) is based on the following result:

Lemma 4.1 *For $X_{0,h} = W^1_{h_t} \otimes V_{h_x}$ and $Y_h = W^0_{h_t} \otimes V_{h_x}$ there holds the discrete inf-sup condition*

$$\|\partial_t u_h\|_{L^2(Q)} \, \leq \, \sup_{0 \neq v_h \in Y_h} \frac{b(u_h, v_h)}{\|v_h\|_{L^2(Q)}} \quad \text{for all } u_h \in X_{0,h}. \tag{4.1}$$

Proof. For $u_h \in X_{0,h} = W^1_{h_t} \otimes V_{h_x}$, we have $\overline{v}_h := \partial_t u_h \in Y_h = W^0_{h_t} \otimes V_{h_x}$, and hence we can write

$$\begin{aligned}
b(u_h, \overline{v}_h) &= \langle \partial_t u_h, \partial_t u_h \rangle_{L^2(Q)} + \langle \nabla_x u_h, \nabla_x \partial_t u_h \rangle_{L^2(Q)} \\
&= \|\partial_t u_h\|^2_{L^2(Q)} + \int_0^T \int_\Omega \nabla_x u_h(x,t) \cdot \nabla_x \partial_t u_h(x,t) \, dx \, dt \\
&= \|\partial_t u_h\|^2_{L^2(Q)} + \frac{1}{2} \int_0^T \frac{d}{dt} \int_\Omega |\nabla_x u_h(x,t)|^2 \, dx \, dt \\
&= \|\partial_t u_h\|^2_{L^2(Q)} + \frac{1}{2} \|\nabla_x u_h(T)\|^2_{L^2(\Omega)} \\
&\geq \|\partial_t u_h\|^2_{L^2(Q)} = \|\partial_t u_h\|_{L^2(Q)} \|\overline{v}_h\|_{L^2(Q)},
\end{aligned}$$

and the assertion follows. ■

While we can use (4.1) to ensure unique solvability of the variational formulation (2.6), we cannot use (4.1) to derive a priori space-time finite element error estimates for the numerical solution $\widetilde{u}_h \in X_{0,h}$. Hence, we will state a different discrete inf-sup condition as follows: When using the temporal piecewise constant L^2 projection $Q^0_{h_t}$ as defined in (3.13), we introduce the mesh dependent norm, similar to the one used in [35],

$$\| u \|_X := \left[c_Q^{-2} \, \|\partial_t u\|^2_{Y^*} + \|Q^0_{h_t} u\|^2_Y \right]^{1/2}, \tag{4.2}$$

where c_Q is the stability constant as used in (3.6).

Lemma 4.2 *For $X_{0,h} = W^1_{h_t} \otimes V_{h_x}$ and $Y_h = W^0_{h_t} \otimes V_{h_x}$, there holds the discrete inf-sup condition*

$$\| u_h \|_X \leq \sup_{0 \neq v_h \in Y_h} \frac{b(u_h, v_h)}{\|v_h\|_Y} \quad \text{for all } u_h \in X_{0,h}. \tag{4.3}$$

Proof. Let $u_h \in X_{0,h} = W^1_{h_t} \otimes V_{h_x}$ be arbitrary but fixed. For $\partial_t u_h \in W^0_{h_t} \otimes V_{h_x} = Y_h$ we determine $w_{u_h,h} \in Y_h$ as the unique solution of the variational formulation

$$\langle \nabla_x w_{u_h,h}, \nabla_x v_h \rangle_{L^2(Q)} = \langle \partial_t u_h, v_h \rangle_{L^2(Q)} \quad \text{for all } v_h \in Y_h. \tag{4.4}$$

It holds that

$$\begin{aligned}
\|\nabla_x w_{u_h,h}\|^2_{L^2(Q)} &= \langle \nabla_x w_{u_h,h}, \nabla_x w_{u_h,h} \rangle_{L^2(Q)} \\
&= \langle \partial_t u_h, w_{u_h,h} \rangle_{L^2(Q)} \leq \|\partial_t u_h\|_{Y^*} \|\nabla_x w_{u_h,h}\|_{L^2(Q)},
\end{aligned}$$

from which $\|w_{u_h,h}\|_Y \leq \|\partial_t u_h\|_{Y^*}$ follows. In order to prove the inverse estimate, we use the definitions and stability estimates for the L^2 projections $Q^1_{h_x}$ and $Q^0_{h_t}$, respectively, to conclude, recall $\partial_t u_h \in Y_h$,

$$\begin{aligned}
\|\partial_t u_h\|_{Y^*} &= \sup_{0\neq v\in Y} \frac{\langle \partial_t u_h, v\rangle_{L^2(Q)}}{\|v\|_Y} = \sup_{0\neq v\in Y} \frac{\langle \partial_t u_h, Q^0_{h_t} Q^1_{h_x} v\rangle_{L^2(Q)}}{\|v\|_Y} \\
&= \sup_{0\neq v\in Y} \frac{\langle \nabla_x w_{u_h,h}, \nabla_x Q^0_{h_t} Q^1_{h_x} v\rangle_{L^2(Q)}}{\|v\|_Y} \\
&\le \sup_{0\neq v\in Y} \frac{\|\nabla_x w_{u_h,h}\|_{L^2(Q)} \|\nabla_x Q^0_{h_t} Q^1_{h_x} v\|_{L^2(Q)}}{\|v\|_Y} \le c_Q \, \|w_{u_h,h}\|_Y .
\end{aligned}$$

For $\overline{v}_h := Q^0_{h_t} u_h + w_{u_h,h} \in Y_h$ we now compute, using (4.4),

$$\begin{aligned}
\|\overline{v}_h\|_Y^2 &= \|Q^0_{h_t} u_h + w_{u_h,h}\|_Y^2 \\
&= \|Q^0_{h_t} u_h\|_Y^2 + \|w_{u_h,h}\|_Y^2 + 2\,\langle w_{u_h,h}, Q^0_{h_t} u_h\rangle_Y \\
&\ge \|Q^0_{h_t} u_h\|_Y^2 + c_Q^{-2}\,\|\partial_t u_h\|_{Y^*}^2 + 2\,\langle \nabla_x w_{u_h,h}, \nabla_x Q^0_{h_t} u_h\rangle_{L^2(Q)} \\
&= \|\!| u_h \|\!|_X^2 + 2\,\langle \partial_t u_h, Q^0_{h_t} u_h\rangle_{L^2(Q)} \\
&= \|\!| u_h \|\!|_X^2 + 2\,\langle \partial_t u_h, u_h\rangle_{L^2(Q)} \ge \|\!| u_h \|\!|_X^2,
\end{aligned}$$

due to

$$\langle \partial_t u_h, u_h\rangle_{L^2(Q)} = \int_\Omega \int_0^T \frac{1}{2}\frac{d}{dt}|u_h(x,t)|^2\,dt\,dx = \frac{1}{2}\int_\Omega |u_h(x,T)|^2\,dx \ge 0.$$

Moreover, we have that

$$\begin{aligned}
b(u_h, \overline{v}_h) &= \langle \partial_t u_h, Q^0_{h_t} u_h + w_{u_h,h}\rangle_{L^2(Q)} + \langle \nabla_x u_h, \nabla_x (Q^0_{h_t} u_h + w_{u_h,h})\rangle_{L^2(Q)} \\
&= \langle \nabla_x w_{u_h,h}, \nabla_x (Q^0_{h_t} u_h + w_{u_h,h})\rangle_{L^2(Q)} + \langle \nabla_x Q^0_{h_t} u_h, \nabla_x (Q^0_{h_t} u_h + w_{u_h,h})\rangle_{L^2(Q)} \\
&= \|\nabla_x (Q^0_{h_t} u_h + w_{u_h,h})\|_{L^2(Q)}^2 = \|\overline{v}_h\|_Y^2 \ge \|\overline{v}_h\|_Y \, \|\!| u_h \|\!|_X,
\end{aligned}$$

which gives the desired result. ■

The stability of the L^2 projection in $H^1_0(\Omega)$ was a sufficient ingredient of the proof. In fact, one can show that it is also necessary, see [34]. We are now in the position to prove a first best approximation result.

Lemma 4.3 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (2.6)*, respectively. Then there holds Cea's lemma,*

$$\|\!| \widetilde{u} - \widetilde{u}_h \|\!|_X \le \sqrt{2}\, c_Q \inf_{z_h \in X_{0,h}} \|\widetilde{u} - z_h\|_X. \tag{4.5}$$

Proof. Let $G_h : X_0 \to X_{0,h}$ denote the Galerkin projection, defined as

$$b(G_h u, v_h) = b(u, v_h), \quad \forall v_h \in Y_h,\ u \in X_0.$$

With the discrete inf-sup condition (4.3) we then conclude

$$\| G_h u \|_X \leq \sup_{0 \neq v_h \in Y_h} \frac{b(G_h u, v_h)}{\|v_h\|_Y} = \sup_{0 \neq v_h \in Y_h} \frac{b(u, v_h)}{\|v_h\|_Y} \leq \sqrt{2}\, c_Q \ \| u \|_X ,$$

where we have used

$$\begin{aligned} b(u, v_h) &= \langle \partial_t u, v_h \rangle_Q + \langle \nabla_x u, \nabla_x v_h \rangle_{L^2(Q)} \\ &= \langle \partial_t u, v_h \rangle_Q + \langle \nabla_x Q^0_{h_t} u, \nabla_x v_h \rangle_{L^2(Q)} \\ &\leq \|\partial_t u\|_{Y^*} \|v_h\|_Y + \|Q^0_{h_t} u\|_Y \|v_h\|_Y \\ &\leq \sqrt{2} \left[\|\partial_t u\|^2_{Y^*} + \|Q^0_{h_t} u\|^2_Y \right]^{1/2} \|v_h\|_Y \leq \sqrt{2}\, c_Q \ \| u \|_X \ \|v_h\|_Y . \end{aligned}$$

■

Moreover, using that $G_h z_h = z_h$ for any $z_h \in X_{0,h}$, $\| u \|_X \leq \|u\|_X$, and $\| (I - G_h) \| = \| G_h \|$, see [9], we have

$$\begin{aligned} \| \widetilde{u} - \widetilde{u}_h \|_X &= \| (I - G_h) \widetilde{u} \|_X = \| (I - G_h)(\widetilde{u} - z_h) \|_X \\ &\leq \| I - G_h \| \, \| \widetilde{u} - z_h \|_X \leq \sqrt{2}\, \|\widetilde{u} - z_h\|_X . \end{aligned}$$

When combining (4.5) with the approximation properties of the space-time finite element space $X_{0,h}$ as given in Lemma 3.1 and Lemma 3.3, we then conclude the following result:

Lemma 4.4 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of (2.4) and (2.6), respectively. Assume $\widetilde{u} \in H^{2,1}(Q) \cap H^2(0,T; H^{-1}(\Omega))$ such that $\nabla_x \partial_t \widetilde{u} \in L^2(Q)$ is satisfied, and let $h_t \simeq h_x$. Then there holds the error estimate*

$$\begin{aligned} \| \widetilde{u} - \widetilde{u}_h \|_X \leq \ & c\, h_x \Big[|\widetilde{u}|^2_{L^2(0,T;H^2(\Omega))} + \|\widetilde{u}\|^2_{H^1(0,T;L^2(\Omega))} \\ & + \|\nabla_x \partial_t \widetilde{u}\|^2_{L^2(Q)} + \|\widetilde{u}\|^2_{H^2(0,T;H^{-1}(\Omega))} \Big]^{1/2} . \end{aligned} \tag{4.6}$$

Proof. We first consider the error estimate (3.15) for $s = 2$ and $\sigma = 1$,

$$\|\widetilde{u} - Q^1_{h_x} I^1_{h_t} \widetilde{u}\|_Y \leq c_1\, h_x\, |\widetilde{u}|_{L^2(0,T;H^2(\Omega))} + c_2\, h_t\, |\widetilde{u}|_{H^1(0,T;H^1_0(\Omega))} ,$$

and the error estimate (3.20) for $\tau = 0$ and $\varrho = 2$, i.e.,

$$\|\partial_t(\widetilde{u} - Q^1_{h_x} I^1_{h_t} \widetilde{u})\|_{Y^*} \leq c_1\, h_x\, \|\widetilde{u}\|_{H^1(0,T;L^2(\Omega))} + c_2\, h_t\, \|\widetilde{u}\|_{H^2(0,T;H^{-1}(\Omega))} .$$

Together with (4.5) for $z_h = Q^1_{h_x} I^1_{h_t} \widetilde{u}$ and choosing $h_t \simeq h_x$ we obtain the assertion. ■

Before we can prove an error estimate for $\|\widetilde{u} - \widetilde{u}_h\|_X$, we need to establish an error estimate for $\|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)}$, as (4.6) only involves the discrete norm $\|Q^0_{h_t}(\widetilde{u} - \widetilde{u}_h)\|_Y$:

Lemma 4.5 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of (2.4) and (2.6), respectively. Assume $\widetilde{u} \in L^2(0,T;H^2(\Omega)) \cap H^2(0,T;L^2(\Omega))$ such that $\partial_t \widetilde{u} \in L^2(0,T;H^2(\Omega))$ and $\widetilde{u} \in H^2(0,T;H^2(\Omega))$ is satisfied. For $h_t \simeq h_x$ there holds the error estimate*

$$\|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)} \, \leq \, c\, h_x^2 \left[\|\widetilde{u}\|_{H^1(0,T;H^2(\Omega))} \, + \, \|\widetilde{u}\|_{H^2(0,T;H^2(\Omega))} \right]. \tag{4.7}$$

Proof. When using the spatial H_0^1 projection $P_{h_x}^1 : H_0^1(\Omega) \to V_{h_x}$ as defined in (3.7), and the piecewise linear temporal interpolation operator $I_{h_t}^1 : H_{0,}^1(0,T) \to W_{h_t}^1$, see (3.11), we can write, using the Galerkin orthogonality

$$\langle \partial_t \widetilde{u}_h, v_h \rangle_Q + \langle \nabla_x \widetilde{u}_h, \nabla_x v_h \rangle_{L^2(Q)} = \langle \partial_t \widetilde{u}, v_h \rangle_Q + \langle \nabla_x \widetilde{u}, \nabla_x v_h \rangle_{L^2(Q)} \tag{4.8}$$

for the particular test function, $v_h = \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \in Y_h$, and using $\partial_t I_{h_t}^1 \widetilde{u} = Q_{h_t}^0 \partial_t \widetilde{u}$,

$$\begin{aligned}
\|\partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u})\|_{L^2(Q)}^2 \; &= \; \langle \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}), \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\leq \; \langle \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}), \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\qquad + \langle \nabla_x(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}), \nabla_x \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&= \; \langle \partial_t(\widetilde{u} - I_{h_t}^1 P_{h_x}^1 \widetilde{u}), \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\qquad + \langle \nabla_x(\widetilde{u} - I_{h_t}^1 \widetilde{u}), \nabla_x \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&= \; \langle \partial_t \widetilde{u} - Q_{h_t}^0 P_{h_x}^1 \partial_t \widetilde{u}, \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\qquad + \langle \nabla_x(\widetilde{u} - I_{h_t}^1 \widetilde{u}), \nabla_x \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&= \; \langle \partial_t \widetilde{u} - P_{h_x}^1 \partial_t \widetilde{u}, \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\qquad + \langle -\Delta_x(\widetilde{u} - I_{h_t}^1 \widetilde{u}), \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}) \rangle_{L^2(Q)} \\
&\leq \; \Big[\|\partial_t \widetilde{u} - P_{h_x}^1 \partial_t \widetilde{u}\|_{L^2(Q)} + \|\Delta_x(\widetilde{u} - I_{h_t}^1 \widetilde{u})\|_{L^2(Q)} \Big] \|\partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u})\|_{L^2(Q)},
\end{aligned}$$

i.e.,

$$\|\partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u})\|_{L^2(Q)} \, \leq \, \|\partial_t \widetilde{u} - P_{h_x}^1 \partial_t \widetilde{u}\|_{L^2(Q)} + \|\Delta_x(\widetilde{u} - I_{h_t}^1 \widetilde{u})\|_{L^2(Q)}\,.$$

For $\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u} \in X_{0,h}$ we can use a Friedrich's type inequality to further obtain

$$\begin{aligned}
\|\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}\|_{L^2(Q)} \; &\leq \; c\, \|\partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u})\|_{L^2(Q)} \\
&\leq \; c \Big[\|\partial_t \widetilde{u} - P_{h_x}^1 \partial_t \widetilde{u}\|_{L^2(Q)} + \|\Delta_x(\widetilde{u} - I_{h_t}^1 \widetilde{u})\|_{L^2(Q)} \Big] \\
&\leq \; c \Big[h_x^2\, |\partial_t \widetilde{u}|_{L^2(0,T;H^2(\Omega))} + h_t^2\, |\Delta_x \widetilde{u}|_{H^2(0,T;L^2(\Omega))} \Big].
\end{aligned}$$

Now the assertion follows from

$$\|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)} \, \leq \, \|\widetilde{u} - I_{h_t}^1 P_{h_x}^1 \widetilde{u}\|_{L^2(Q)} + \|\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1 \widetilde{u}\|_{L^2(Q)},$$

when using, see also the proof of (3.15),

$$\begin{aligned}\|\widetilde{u} - I^1_{h_t} P^1_{h_x} \widetilde{u}\|_{L^2(Q)} &\leq \|\widetilde{u} - P^1_{h_x}\widetilde{u}\|_{L^2(Q)} + \|(\widetilde{u} - I^1_{h_t}\widetilde{u}) P^1_{h_x}\|_{L^2(Q)} \\ &\leq c_1\, h_x^2\, \|\widetilde{u}\|_{L^2(0,T;H^2(\Omega))} + c_2\, h_t^2\, \|\widetilde{u}\|_{H^2(0,T;L^2(\Omega))}\,.\end{aligned}$$

■

Theorem 4.6 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (2.6)*, respectively. For $\widetilde{u}$ let all assumptions of Lemma* 4.5 *be valid. Then there holds the error estimate*

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq c(\widetilde{u})\, h_x, \tag{4.9}$$

where $c(\widetilde{u})$ covers all contributions as given in (4.7)*.*

Proof. We first note that

$$\|\widetilde{u} - \widetilde{u}_h\|^2_X = \|\partial_t(\widetilde{u} - \widetilde{u}_h)\|^2_{Y^*} + \|\widetilde{u} - \widetilde{u}_h\|^2_Y \leq \|\partial_t(\widetilde{u} - \widetilde{u}_h)\|^2_{L^2(Q)} + \|\widetilde{u} - \widetilde{u}_h\|^2_Y.$$

When using the spatial H^1_0 projection $P^1_{h_x} : H^1_0(\Omega) \to V_{h_x} \subset H^1_0(\Omega)$ and the temporal piecewise linear interpolation $I^1_{h_t}$ as defined in (3.11), we obtain

$$\|\partial_t(\widetilde{u} - \widetilde{u}_h)\|_{L^2(Q)} \leq \|\partial_t(\widetilde{u} - I^1_{h_t} P^1_{h_x}\widetilde{u})\|_{L^2(Q)} + \|\partial_t(I^1_{h_t} P^1_{h_x}\widetilde{u}) - \widetilde{u}_h\|_{L^2(Q)},$$

and as in the proof of Lemma 4.5, we get, recall $h_t \sim h_x$,

$$\begin{aligned}\|\partial_t(I^1_{h_t} P^1_{h_x}\widetilde{u} - \widetilde{u}_h)\|_{L^2(Q)} &\leq \|\partial_t\widetilde{u} - P^1_{h_x}\partial_t\widetilde{u}\|_{L^2(Q)} + \|\Delta_x(\widetilde{u} - I^1_{h_t}\widetilde{u})\|_{L^2(Q)} \\ &\leq c\, h_x \Big(\|\widetilde{u}\|_{H^1(0,T;H^1(\Omega))} + \|\widetilde{u}\|_{H^1(0,T;H^2(\Omega))}\Big).\end{aligned}$$

Moreover, using $\partial_t I^1_{h_t}\widetilde{u} = Q^0_{h_t}\partial_t\widetilde{u}$, and the error estimates (3.14) and (3.10), we compute

$$\begin{aligned}\|\partial_t(\widetilde{u} - I^1_{h_t} P^1_{h_x}\widetilde{u})\|_{L^2(Q)} &= \|\partial_t\widetilde{u} - Q^0_{h_t} P^1_{h_x}\partial_t\widetilde{u}\|_{L^2(Q)} \\ &\leq \|\partial_t\widetilde{u} - Q^0_{h_t}\partial_t\widetilde{u}\|_{L^2(Q)} + \|Q^0_{h_t}(\partial_t\widetilde{u} - P^1_{h_x}\partial_t\widetilde{u})\|_{L^2(Q)} \\ &\leq c\, h_t\, \|\partial_{tt}\widetilde{u}\|_{L^2(Q)} + \|\partial_t\widetilde{u} - P^1_{h_x}\partial_t\widetilde{u}\|_{L^2(Q)} \\ &\leq c\, h_x \Big(\|\widetilde{u}\|_{H^2(0,T;L^2(\Omega))} + \|\widetilde{u}\|_{H^1(0,T;H^1(\Omega))}\Big).\end{aligned}$$

Together with the estimate

$$\begin{aligned}\|\widetilde{u} - \widetilde{u}_h\|_Y &\leq \|\nabla_x(\widetilde{u} - P^1_{h_x}\widetilde{u})\|_{L^2(Q)} + \|\nabla_x(P^1_{h_x}\widetilde{u} - \widetilde{u}_h)\|_{L^2(Q)} \\ &\leq \|\nabla_x(\widetilde{u} - P^1_{h_x}\widetilde{u})\|_{L^2(Q)} + c\, h_x^{-1}\, \|P^1_{h_x}\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)} \\ &\leq \|\nabla_x(\widetilde{u} - P^1_{h_x}\widetilde{u})\|_{L^2(Q)} + c\, h_x^{-1} \Big[\|P^1_{h_x}\widetilde{u} - \widetilde{u}\|_{L^2(Q)} + \|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)}\Big],\end{aligned}$$

and using the error estimates (3.9) and (3.10) gives the assertion (4.9). ■

Since all of the above error estimates (4.6), (4.7), and (4.9) require a sufficiently regular solution $\widetilde{u}$, we now aim to derive error estimates for less regular solutions. To do so, we first establish a discrete inf-sup condition in the norm $\|u_h\|_X$ being an equivalent norm to $\|\!| u_h \|\!|_X$ for $u_h \in X_{0,h}$. From (4.2) we already have that $\|\!| u_h \|\!|_X \leq \max\{1, c_Q^{-1}\} \|u_h\|_X$ for all $u_h \in X_{0,h}$. Now we will show the reverse inequality, that is also outlined in [2, (5.2.63)].

Lemma 4.7 *For any $u_h \in X_{0,h}$, there holds*

$$\|\!| u_h \|\!|_X \geq c \min\{1, h_t^{-1} h_x^2\} \|u_h\|_X . \tag{4.10}$$

Proof. When using the Galerkin orthogonality and the error estimate (3.14) for the temporal L^2 projection $Q^0_{h_t}$, and the inverse inequality (3.1) together with a duality argument, we first compute

$$\begin{aligned}
\|u_h\|_Y^2 &= \|\nabla_x Q^0_{h_t} u_h\|^2_{L^2(Q)} + \|\nabla_x (I - Q^0_{h_t}) u_h\|^2_{L^2(Q)} \\
&\leq \|Q^0_{h_t} u_h\|_Y^2 + c\, h_t^2 \, \|\partial_t u_h\|^2_{L^2(0,T;H^1_0(\Omega))} \\
&\leq \|Q^0_{h_t} u_h\|_Y^2 + c\ h_t^2 \, h_x^{-4} \, \|\partial_t u_h\|^2_{L^2(0,T;H^{-1}(\Omega))}.
\end{aligned}$$

So, we get

$$\begin{aligned}
\|u_h\|_X^2 &= \|\partial_t u_h\|^2_{Y^*} + \|u_h\|_Y^2 \\
&\leq \|Q^0_{h_t} u_h\|_Y^2 + \Big[1 + c\, h_t^2 \, h_x^{-4}\Big] \|\partial_t u_h\|^2_{Y^*} \\
&\leq \max\{c_Q^2, 1 + c\, h_t^2\, h_x^{-4}\} \Big[c_Q^{-2} \, \|Q^0_{h_t} u_h\|_Y^2 + \|\partial_t u_h\|^2_{Y^*}\Big],
\end{aligned}$$

and the assertion follows. ■

When combining the discrete inf-sup stability condition (4.3) and the norm equivalence inequality (4.10), this results in the discrete inf-sup stability condition

$$c_{S,h} \, \|u_h\|_X \leq \sup_{0 \neq v_h \in Y_h} \frac{b(u_h, v_h)}{\|v_h\|_Y} \quad \text{for all } u_h \in X_{0,h}, \tag{4.11}$$

where $c_{S,h} := c \min\{1, h_t^{-1} h_x^2\}$. In particular we then conclude the Cea type estimate

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq \frac{\sqrt{2}}{c_{S,h}} \inf_{z_h \in X_{0,h}} \|\widetilde{u} - z_h\|_X. \tag{4.12}$$

Remark 4.1 *Even for smooth solutions $\widetilde{u}$, the quasi best approximation error is at best*

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq \frac{\sqrt{2}}{c_{S,h}} \inf_{z_h \in X_{0,h}} \|\widetilde{u} - z_h\|_X \leq \frac{\sqrt{2}}{c_{S,h}} h_x \, c(\widetilde{u}).$$

In the case of orthotropic scaling, i.e., $h_t \simeq h_x$, we have $c_{S,h} \simeq h_x$, which would suggest that no convergence is observed. However, in (4.9) *we derived an estimate of order h_x in this setting. This indicates that for $\widetilde{u}$ satisfying the assumption of Lemma 4.5, the discrete inf-sup constant exhibits the behavior $c_{S,h} = c_{S,h}(\widetilde{u}) \simeq 1$, i.e., it improves on a certain subclass U of functions $\widetilde{u} \in U \subset X_0$, see also* [5].

On the other hand, for parabolic scaling $h_t \simeq h_x^2$, we have $c_{S,h} \simeq 1$, and with the approximation properties of the space-time finite element space $X_{0,h}$ we obtain the following result:

Lemma 4.8 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (2.6)*, respectively. Assume $\widetilde{u} \in H^{2,1}(Q) \cap H^{3/2}(0,T;H^{-1}(\Omega))$. For $h_t \simeq h_x^2$ there holds the error estimate*

$$\|\widetilde{u} - \widetilde{u}_h\|_X \,\leq\, c\, h_x \left[\|\widetilde{u}\|^2_{H^{2,1}(Q)} + \|\widetilde{u}\|^2_{H^{3/2}(0,T;H^{-1}(\Omega))} \right]^{1/2} . \tag{4.13}$$

Proof. We first consider the error estimate (3.16) for $s = 2$ and $\sigma = 1$,

$$\|\widetilde{u} - Q^1_{h_x} I^1_{h_t} \widetilde{u}\|_Y \,\leq\, c_1\, h_x\, \|\widetilde{u}\|_{L^2(0,T;H^2(\Omega))} + c_2\, h_x^{-1}\, h_t\, \|\widetilde{u}\|_{H^1(0,T;L^2(\Omega))},$$

and the error estimate (3.20) for $\tau = 0$ and $\varrho = 3/2$,

$$\|\widetilde{u} - \widetilde{u}_h\|_{Y^*} \,\leq\, c_1\, h_x\, \|\partial_t \widetilde{u}\|_{L^2(Q)} + c_2\, h_t^{1/2}\, \|\widetilde{u}\|_{H^{3/2}(0,T;H^{-1}(\Omega))} .$$

In particular for $h_t \simeq h_x^2$ and using (4.12) for $z_h = Q^1_{h_x} I^1_{h_t} \widetilde{u}$, the assertion follows. ∎

Similar as for second order elliptic problems, for smoothly bounded or convex spatial domains Ω, we can now use the Nitsche trick to conclude an error estimate in $L^2(Q)$.

Lemma 4.9 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (2.6)*, respectively. For $h_t \simeq h_x^2$ there holds the error estimate*

$$\|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)} \,\leq\, c\, h_x\, \|\widetilde{u} - \widetilde{u}_h\|_X \, . \tag{4.14}$$

Proof. Let us consider the adjoint heat equation,

$$\begin{array}{rcll} -\partial_t p(x,t) - \Delta_x p(x,t) & = & \widetilde{u}(x,t) - \widetilde{u}_h(x,t) & \text{for } (x,t) \in Q, \\ p(x,t) & = & 0 & \text{for } (x,t) \in \Sigma, \\ p(x,T) & = & 0 & \text{for } x \in \Omega, \end{array}$$

i.e., $p \in Y$ is the unique solution of the variational formulation

$$b(w,p) \,=\, \langle \widetilde{u} - \widetilde{u}_h, w \rangle_{L^2(Q)} \quad \text{for all } w \in X_0 \, .$$

In particular for $w = \widetilde{u} - \widetilde{u}_h \in X_0$ this gives

$$\begin{array}{rcl} \|\widetilde{u} - \widetilde{u}_h\|^2_{L^2(Q)} & = & \langle \widetilde{u} - \widetilde{u}_h, \widetilde{u} - \widetilde{u}_h \rangle_{L^2(Q)} \,=\, b(\widetilde{u} - \widetilde{u}_h, p) \\ & = & b(\widetilde{u} - \widetilde{u}_h, p - Q^1_{h_x} Q^0_{h_t} p) \,\leq\, \sqrt{2}\, \|\widetilde{u} - \widetilde{u}_h\|_X \|p - Q^1_{h_x} Q^0_{h_t} p\|_Y \, . \end{array}$$

By parabolic regularity we have that $p \in H^{2,1}(Q)$, since $\widetilde{u} - \widetilde{u}_h \in L^2(Q)$, see (4.13). Next we use the error estimate (3.19) for $s = 2$ and $\sigma = 1$,

$$\|p - Q^1_{h_x} Q^0_{h_t} p\|_Y \,\leq\, c_1\, h_x\, |p|_{L^2(0,T;H^2(\Omega))} + c_2\, h_x^{-1}\, h_t\, \|p\|_{H^1(0,T;L^2(\Omega))} \,\leq\, c\, h_x\, \|p\|_{H^{2,1}(Q)},$$

when choosing $h_t \simeq h_x^2$. Now the assertion follows from the regularity estimate (A.15),

$$\|p\|_{H^{2,1}(Q)} \leq \|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)},$$

and the error estimate (4.13). ∎

Now we are in the position to consider the case when the initial datum u_0 is discontinuous. For this we consider the homogeneous heat equation (1.1) with $f \equiv 0$, where we can reformulate the previous error estimates as follows.

Theorem 4.10 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (2.6)*, respectively. Assume $f \equiv 0$, and $u_0 \in \widetilde{H}^s(\Omega) := [L^2(\Omega), H_0^1(\Omega)]_{|s}$ for some $s \in [0,1]$. For $h_t \simeq h_x^2$ there hold the error estimates*

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq c\, h_x^s\, \|u_0\|_{\widetilde{H}^s(\Omega)}, \tag{4.15}$$

and

$$\|\widetilde{u} - \widetilde{u}_h\|_{L^2(Q)} \leq c\, h_x^{1+s}\, \|u_0\|_{\widetilde{H}^s(\Omega)}. \tag{4.16}$$

Proof. For $f \equiv 0$ and assuming $u_0 \in H_0^1(\Omega)$, the error estimate (4.13) reads

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq h_x \left[\|\widetilde{u}\|^2_{H^{2,1}(Q)} + \|\widetilde{u}\|^2_{H^{3/2}(0,T;H^{-1}(Q))} \right]^{1/2} \leq c\, h_x\, \|\nabla_x u_0\|_{L^2(\Omega)},$$

while using (4.12) for $z_h = 0$ and the regularity estimate (A.3) this gives

$$\|\widetilde{u} - \widetilde{u}_h\|_X \leq c\, \|\widetilde{u}\|_X \leq c\, \|u_0\|_{L^2(\Omega)}.$$

Now, (4.15) follows from a space interpolation argument, and (4.16) follows as in the proof of (4.14). ∎

All of the previous error estimates are formulated for the solution $\widetilde{u}_h$ satisfying the finite element variational formulation (2.6), which involves the extension $\widetilde{u}_0$ of the given initial datum u_0. Hence, and as in the case of Dirichlet boundary conditions for elliptic problems, we proceed as follows. For $\widetilde{u}_0 \in X$ we consider the space-time finite element approximation $I^1_{h_t} Q^1_{h_x} \widetilde{u}_0$, and instead of (2.6) we consider a perturbed variational formulation to find $\widetilde{u}_h^* \in X_{0,h}$ such that

$$b(\widetilde{u}_h^* + I^1_{h_t} Q^1_{h_x} \widetilde{u}_0, v_h) = \langle f, v_h \rangle_Q \quad \text{for all } v_h \in Y_h, \tag{4.17}$$

and subtracting (4.17) from (2.6) gives the perturbed Galerkin orthogonality

$$b(\widetilde{u}_h - \widetilde{u}_h^*, v_h) = b(I^1_{h_t} Q^1_{h_x} \widetilde{u}_0 - \widetilde{u}_0, v_h) \quad \text{for all } v_h \in Y_h. \tag{4.18}$$

As in the elliptic case we can use the Strang lemma to analyse this additional error:

Lemma 4.11 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h^* \in X_{0,h}$ denote the unique solutions of (2.4) and (4.17), respectively. Assume $\widetilde{u}, \widetilde{u}_0 \in H^{2,1}(Q) \cap H^2(0,T;H^{-1}(\Omega))$ such that $\nabla_x \partial_t \widetilde{u}, \nabla_x \partial_t \widetilde{u}_0 \in L^2(Q)$ are satisfied, and let $h_t \simeq h_x$. Then there holds the error estimate*

$$\| \widetilde{u} - \widetilde{u}_h^* \|_X \leq c(\widetilde{u}, \widetilde{u}_0)\, h_x \,. \tag{4.19}$$

If $\widetilde{u}, \widetilde{u}_0 \in L^2(0,T;H^2(\Omega)) \cap H^2(0,T;L^2(\Omega))$ and $\partial_t \widetilde{u}, \partial_t \widetilde{u}_0 \in L^2(0,T;H^2(\Omega))$ as well as $\Delta_x \widetilde{u}, \Delta_x \widetilde{u}_0 \in H^2(0,T;L^2(\Omega))$ is satisfied, then

$$\|\widetilde{u} - \widetilde{u}_h^*\|_{L^2(Q)} \,\leq\, c(\widetilde{u}, \widetilde{u}_0)\, h_x^2 \,, \tag{4.20}$$

and

$$\|\widetilde{u} - \widetilde{u}_h^*\|_Y \,\leq\, c(\widetilde{u}, \widetilde{u}_0)\, h_x \,. \tag{4.21}$$

Proof. By the triangle inequality we first have

$$\| \widetilde{u} - \widetilde{u}_h^* \|_X \leq \| \widetilde{u} - \widetilde{u}_h \|_X + \| \widetilde{u}_h - \widetilde{u}_h^* \|_X,$$

and with (4.3) we further obtain

$$\begin{aligned} \| \widetilde{u}_h - \widetilde{u}_h^* \|_X &\leq \sup_{0 \neq v_h \in Y_h} \frac{b(\widetilde{u}_h - \widetilde{u}_h^*, v_h)}{\|v_h\|_Y} \\ &= \sup_{0 \neq v_h \in Y_h} \frac{b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, v_h)}{\|v_h\|_Y} \\ &\leq \sqrt{2}\, \|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_X \,=\, \sqrt{2}\, \|\widetilde{u}_0 - Q_{h_x}^1 I_{h_t}^1 \widetilde{u}_0\|_X, \end{aligned}$$

since the nodal temporal interpolation $I_{h_t}^1$ and the spatial L^2 projection $Q_{h_x}^1$ commute. Hence we can use the error estimates (3.15) and (3.20) to conclude (4.19). In order to estimate $\|\widetilde{u} - \widetilde{u}_h^*\|_{L^2(Q)}$ we can proceed as in the proof of Lemma 4.5. But instead of (4.8) we have to use the perturbed Galerkin orthogonality

$$b(\widetilde{u}_h^*, v_h) \,=\, b(\widetilde{u}, v_h) + b(\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0, v_h)$$

for the particular test function $v_h = \partial_t(\widetilde{u}_h - I_{h_t}^1 P_{h_x}^1)\widetilde{u} \in Y_h$. In any case, the additional term can be estimated similar as in the proof of Lemma 4.5 to conclude (4.20). The error estimate (4.21) finally follows as in Theorem 4.6. ∎

It remains to consider error estimates for the solution $\widetilde{u}_h^*$ of the perturbed variational formulation (4.17), when the solution $\widetilde{u}$ is less regular, and parabolic scaling $h_t \simeq h_x^2$ is required.

Lemma 4.12 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h^* \in X_{0,h}$ denote the unique solutions of (2.4) and (4.17), respectively. Assume $\widetilde{u}, \widetilde{u}_0 \in H^{2,1}(Q) \cap H^{3/2}(0,T;H^{-1}(\Omega))$. For $h_t \simeq h_x^2$ there holds*

$$\|\widetilde{u} - \widetilde{u}_h^*\|_X \,\leq\, \|\widetilde{u} - \widetilde{u}_h\|_X + c\, \|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_X, \tag{4.22}$$

and

$$\begin{aligned} \|\widetilde{u} - \widetilde{u}_h^*\|_{L^2(Q)} \,\leq\, & c\, h_x \Big[\|\widetilde{u} - \widetilde{u}_h^*\|_X + \|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_X \Big] \\ & + \|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_{L^2(Q)} \,+\, \|u_0 - Q_{h_x}^1 u_0\|_{L^2(\Omega)}. \end{aligned} \tag{4.23}$$

Proof. As in the proof of Lemma 4.11 we first have

$$\|\widetilde{u}-\widetilde{u}_h^*\|_X \,\leq\, \|\widetilde{u}-\widetilde{u}_h\|_X + \|\widetilde{u}_h-\widetilde{u}_h^*\|_X,$$

but now we use (4.11) for $h_t \simeq h_x^2$ and (4.18) to conclude

$$\begin{aligned} c\,\|\widetilde{u}_h-\widetilde{u}_h^*\|_X &\leq \sup_{0\neq v_h\in Y_h} \frac{b(\widetilde{u}_h-\widetilde{u}_h^*,v_h)}{\|v_h\|_Y} \\ &= \sup_{0\neq v_h\in Y_h} \frac{b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0-\widetilde{u}_0,v_h)}{\|v_h\|_Y} \,\leq\, \sqrt{2}\,\|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_X . \end{aligned}$$

To prove (4.23), we can proceed as in the proof of Lemma 4.9, but now we obtain

$$\begin{aligned} \|\widetilde{u}-\widetilde{u}_h^*\|^2_{L^2(Q)} &= \langle \widetilde{u}-\widetilde{u}_h^*, \widetilde{u}-\widetilde{u}_h^*\rangle_{L^2(Q)} \,=\, b(\widetilde{u}-\widetilde{u}_h^*,p) \\ &= b(\widetilde{u}-\widetilde{u}_h^*, p - Q_{h_x}^1 Q_{h_t}^0 p) + b(\widetilde{u}-\widetilde{u}_h^*, Q_{h_x}^1 Q_{h_t}^0 p) \\ &= b(\widetilde{u}-\widetilde{u}_h^*, p - Q_{h_x}^1 Q_{h_t}^0 p) + b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, Q_{h_x}^1 Q_{h_t}^0 p), \end{aligned}$$

and it remains to consider the second term,

$$\begin{aligned} & b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, Q_{h_x}^1 Q_{h_t}^0 p) \\ &\quad = b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, Q_{h_x}^1 Q_{h_t}^0 p - p) + b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, p) \\ &\quad \leq \sqrt{2}\,\|\widetilde{u}_0 - I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0\|_X \|p - Q_{h_x}^1 Q_{h_t}^0 p\|_Y + b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, p), \end{aligned}$$

and the first part can be further estimated as in the proof of Lemma 4.9. Using integration by parts in space and time we obtain

$$\begin{aligned} b(I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, p) &= \langle \partial_t (I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0), p\rangle_Q + \langle \nabla_x (I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0), \nabla_x p\rangle_{L^2(Q)} \\ &= \langle I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0, -\partial_t p - \Delta_x p\rangle_{L^2(Q)} - \langle Q_{h_x}^1 u_0 - u_0, p(0)\rangle_{L^2(\Omega)} \\ &\leq \Big[\|I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 - \widetilde{u}_0\|_{L^2(Q)} + \|u_0 - Q_{h_x}^1 u_0\|_{L^2(\Omega)} \Big] \|p\|_{H^{2,1}(Q)}, \end{aligned}$$

and the assertion follows. ∎

When combining the results of Theorem 4.10 and Lemma 4.12 we finally conclude:

Theorem 4.13 *Let $\widetilde{u} \in X_0$ and $\widetilde{u}_h^* \in X_{0,h}$ denote the unique solutions of* (2.4) *and* (4.17), *respectively. Assume $f \equiv 0$, and $u_0 \in \widetilde{H}^s(\Omega) := [L^2(\Omega), H^1_0(\Omega)]_{|s}$ for some $s \in [0,1]$. For $h_t \simeq h_x^2$ there hold the error estimates*

$$\|\widetilde{u}-\widetilde{u}_h^*\|_X \,\leq\, c\,h_x^s\,\|u_0\|_{\widetilde{H}^s(\Omega)}, \tag{4.24}$$

and

$$\|\widetilde{u}-\widetilde{u}_h^*\|_{L^2(Q)} \,\leq\, c\,h_x^{1+s}\,\|u_0\|_{\widetilde{H}^s(\Omega)}. \tag{4.25}$$

By introducing

$$u_h := \widetilde{u}_h^* + I_{h_t}^1 Q_{h_x}^1 \widetilde{u}_0 = \sum_{i=0}^{N_t} \sum_{k=1}^{M_x} u_k^i \, \psi_i^1(t) \, \varphi_k(x)$$

we can write the variational formulation (4.17) as

$$b(u_h, v_h) = \langle f, v_h \rangle_Q \quad \text{for all } v_h \in Y_h.$$

For the particular test function $v_h(x,t) = \psi_i^0(t)\varphi_\ell(x)$, $i = 1, \ldots, N_t$, $\ell = 1, \ldots, M_x$, this gives

$$\begin{aligned}
&\sum_{k=1}^{M_x} \int_{t_{i-1}}^{t_i} \frac{u_k^i - u_k^{i-1}}{h_t} \, dt \int_\Omega \varphi_k(x) \, \varphi_\ell(x) \, dx \\
&\quad + \sum_{k=1}^{M_x} \int_{t_{i-1}}^{t_i} \left(u_k^{i-1} + \frac{t - t_{i-1}}{h_t} (u_k^i - u_k^{i-1}) \right) \, dt \int_\Omega \nabla_x \varphi_k(x) \cdot \nabla_x \varphi_\ell(x) \, dx \\
&\qquad\qquad = \int_{t_{i-1}}^{t_i} f(x,t) \varphi_\ell(x) \, dx \, ,
\end{aligned}$$

which is equivalent to the algebraic system of linear equations,

$$M_h(\underline{u}^i - \underline{u}^{i-1}) + \frac{1}{2} h_t \, K_h(\underline{u}^i + \underline{u}^{i-1}) \; = \; \underline{f}^i \, , \quad i = 1, \ldots, N_t. \tag{4.26}$$

Despite the different evaluation of the right hand side $\underline{f}^i$ this is the Crank–Nicolson scheme, which was introduced in [10], to *remove the oscillatory behavior and allow for much bigger time-steps* than in a method proposed before by Richardson [27]. Note that the coefficients $\underline{u}^0$ are determined from the L^2 projection of the initial datum u_0. But it is well known that a piecewise linear continuous approximation of a discontinuous initial datum u_0 produces oscillations around the discontinuity, see also the discussion in [36]. This motivates the following considerations.

5 The adjoint space-time FEM for the heat equation

When considering the variational formulation (2.1), and using integration by parts in time, this gives

$$\begin{aligned}
\int_0^T \int_\Omega f(x,t) \, v(x,t) \, dx \, dt \;\; &= \;\; \int_0^T \int_\Omega \Big[\partial_t u(x,t) \, v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t) \Big] \, dx \, dt \\
&= \int_0^T \int_\Omega \Big[- u(x,t) \, \partial_t v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t) \Big] \, dx \, dt - \int_\Omega u_0(x) \, v(x,0) \, dx
\end{aligned}$$

when using $v(x,T) = 0$, $x \in \Omega$. Hence we conclude a variational formulation to find $u \in Y = L^2(0,T;H^1_0(\Omega))$ such that

$$b_T(u,v) := \int_0^T \int_\Omega \Big[- u(x,t)\, \partial_t v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t) \Big]\, dx\, dt \tag{5.1}$$
$$= \int_0^T \int_\Omega f(x,t)\, v(x,t)\, dx\, dt + \int_\Omega u_0(x)\, v(x,0)\, dx$$

is satisfied for all $v \in X_T := \{v \in X : v(x,T) = 0, x \in \Omega\}$. Unique solvability of (5.1) follows as in the case of the primal variational formulation (2.1), see also [24, Lemma 3.1].

For the discretization of (5.1) we use the ansatz space $Y_h = W^0_{h_t} \otimes V_{h_x}$ of functions which are piecewise linear in space but piecewise constant in time, and the test space $X_{T,h} = \overline{W}^1_{h_t} \otimes V_{h_x}$, where $\overline{W}^1_{h_t} = \mathrm{span}\{\psi^1_i\}_{i=0}^{N_t-1} \subset H^1_{,0}(0,T)$ is the space of piecewise linear continuous functions which are zero at $t = T$. Then we determine $u_h \in Y_h$ such that

$$b_T(u_h, v_h) = \langle f, v_h \rangle_Q + \langle u_0, v_h(0) \rangle_{L^2(\Omega)} \quad \text{for all } v_h \in X_{T,h}. \tag{5.2}$$

Unique solvability of (5.2) is a direct consequence of the discrete inf-sup condition (4.11).

Lemma 5.1 *For $Y_h = W^0_{h_t} \otimes V_{h_x}$ and $X_{T,h} = \overline{W}^1_{h_t} \otimes V_{h_x}$ there holds the discrete inf-sup stability condition*

$$c_{S,h}\, \|u_h\|_Y \le \sup_{0 \neq v_h \in X_{T,h}} \frac{b_T(u_h, v_h)}{\|v_h\|_X} \quad \textit{for all } u_h \in Y_h, \tag{5.3}$$

where $c_{S,h} = c\, \min\{1, h_t^{-1}\, h_x^2\}$.

Proof. Consider the time reversal operator $\iota_T v(t) = v(T-t)$, which is an isometry. For any given $u_h \in Y_h$ we first compute $\overline{v}_h \in X_{0,h} = \iota_T(X_{T,h})$ as unique solution of the variational formulation

$$b(\overline{v}_h, \iota_T w_h) = \langle \nabla_x \iota_T u_h, \nabla_x \iota_T w_h \rangle_{L^2(Q)} \quad \text{for all } w_h \in Y_h,$$

and using the discrete inf-sup stability condition (4.11) this gives

$$\begin{aligned} c\, \min\{1, h_t^{-1}\, h_x^2\}\, \|\overline{v}_h\|_X &\le \sup_{0 \neq w_h \in Y_h} \frac{b(\overline{v}_h, \iota_T w_h)}{\|w_h\|_Y} \\ &= \sup_{0 \neq w_h \in Y_h} \frac{\langle \nabla_x \iota_T u_h, \nabla_x \iota_T w_h \rangle_{L^2(Q)}}{\|w_h\|_Y} \le \|\iota_T u_h\|_Y = \|u_h\|_Y. \end{aligned}$$

Now let $\widehat{v}_h(t) := \iota_T \overline{v}_h(t)$, $t \in (0,T)$, then we can write, see Lemma B.1,

$$\begin{aligned} b_T(u_h, \widehat{v}_h) &= b(\overline{v}_h, \iota_T u_h) = \langle \nabla_x \iota_T u_h, \nabla_x \iota_T u_h \rangle_{L^2(Q)} \\ &= \|u_h\|_Y^2 \ge c\, \min\{1, h_t^{-1}\, h_x^2\}\, \|u_h\|_Y \|\overline{v}_h\|_X, \end{aligned}$$

implying the assertion, noting that $\|\overline{v}_h\|_X = \|\widehat{v}\|_X$. ∎

Remark 5.1 *In fact, one can show that the discrete inf-sup constants for the primal and the adjoint problem are equal, see Lemma B.1, i.e.,*

$$\inf_{u_h \in X_{0,h}} \sup_{0 \neq v_h \in Y_h} \frac{b(u_h, v_h)}{\|u_h\|_X \|v_h\|_Y} = \inf_{v_h \in Y_h} \sup_{0 \neq u_h \in X_{T,h}} \frac{b_T(v_h, u_h)}{\|v_h\|_Y \|u_h\|_X}.$$

Thus, we assume if u satisfies the assumption of Lemma 4.5*, we again have in the case of orthotropic scaling $h_t \simeq h_x$ that $c_{S,h} \simeq 1$.*

As a direct consequence of the discrete inf-sup stability condition (5.3), and as in (4.12), we conclude Cea's lemma

$$\|u - u_h\|_Y \ \le\ \frac{\sqrt{2}}{c_{S,h}} \inf_{w_h \in Y_h} \|u - w_h\|_Y \,. \tag{5.4}$$

When combining this with the error estimate (3.19) for $s = 2$ and $\sigma = 1$, we conclude the following result:

Theorem 5.2 *Let $u \in Y$ and $u_h \in Y_h$ be the unique solutions of the variational formulations* (5.1) *and* (5.2)*, respectively. Assume $u \in H^{2,1}(Q)$, and let $h_t \simeq h_x^2$, or let u satisfy all the assumptions of Lemma* 4.5*. Then there holds the error estimate*

$$\|u - u_h\|_Y \ \le\ c\, h_x \, |u|_{H^{2,1}(Q)}. \tag{5.5}$$

It remains to derive an estimate for the error in $L^2(Q)$:

Lemma 5.3 *For $u \in Y$ and $u_h \in Y_h$ being the unique solutions of the variational problems* (5.1) *and* (5.2)*, there holds the error estimate*

$$\|u - u_h\|_{L^2(Q)} \ \le\ c \Big[\|u - P^1_{h_x} u\|_{L^2(Q)} + \|u - Q^0_{h_t} u\|_{L^2(Q)} + h_x^{-1}\, h_t \, \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)} \Big]. \tag{5.6}$$

Proof. From the variational formulations (5.1) and (5.2) we first conclude the Galerkin orthogonality

$$-\langle u_h, \partial_t v_h \rangle_Q + \langle \nabla_x u_h, \nabla_x v_h \rangle_{L^2(Q)} \ =\ -\langle u, \partial_t v_h \rangle_Q + \langle \nabla_x u, \nabla_x v_h \rangle_{L^2(Q)}, \quad v_h \in X_{T,h}.$$

For $w_h \in Y_h$, define

$$\overline{v}_h(x,t) := \int_t^T w_h(x,s)\, ds, \quad \overline{v}_h \in X_{T,h}, \quad \partial_t \overline{v}_h(x,t) = -w_h(x,t),$$

where we have

$$\begin{aligned} \int_0^T \int_\Omega \nabla_x w_h(x,t) \cdot \nabla_x \overline{v}_h(x,t)\, dx\, dt \ &=\ - \int_0^T \int_\Omega \nabla_x \partial_t \overline{v}_h(x,t) \cdot \nabla_x \overline{v}_h(x,t)\, dx\, dt \\ &=\ -\frac{1}{2} \int_0^T \frac{d}{dt} \int_\Omega |\nabla_x \overline{v}_h(x,t)|^2\, dx\, dt \\ &=\ -\frac{1}{2} \, \|\nabla_x \overline{v}_h(t)\|^2_{L^2(\Omega)} \Big|_0^T \ =\ \frac{1}{2} \, \|\nabla_x \overline{v}_h(0)\|^2_{L^2(\Omega)} \ \ge\ 0. \end{aligned}$$

In particular for $w_h = u_h - P^1_{h_x} Q^0_{h_t} u \in Y_h$ we can write

$$\begin{aligned}
\|u_h - P^1_{h_x} Q^0_{h_t} u\|^2_{L^2(Q)} &= \langle u_h - P^1_{h_x} Q^0_{h_t} u, u_h - P^1_{h_x} Q^0_{h_t} u\rangle_{L^2(Q)} \\
&= -\langle u_h - P^1_{h_x} Q^0_{h_t} u, \partial_t \overline{v}_h\rangle_{L^2(Q)} \\
&\leq -\langle u_h - P^1_{h_x} Q^0_{h_t} u, \partial_t \overline{v}_h\rangle_{L^2(Q)} + \langle \nabla_x (u_h - P^1_{h_x} Q^0_{h_t} u), \nabla_x \overline{v}_h\rangle_{L^2(Q)} \\
&= -\langle u - P^1_{h_x} Q^0_{h_t} u, \partial_t \overline{v}_h\rangle_{L^2(Q)} + \langle \nabla_x (u - P^1_{h_x} Q^0_{h_t} u), \nabla_x \overline{v}_h\rangle_{L^2(Q)}.
\end{aligned}$$

For the first term we have

$$\begin{aligned}
-\langle u - P^1_{h_x} Q^0_{h_t} u, \partial_t \overline{v}_h\rangle_{L^2(Q)} &= -\langle u - P^1_{h_x} u, \partial_t \overline{v}_h\rangle_{L^2(Q)} \\
&\leq \|u - P^1_{h_x} u\|_{L^2(Q)} \|\partial_t \overline{v}_h\|_{L^2(Q)} \\
&= \|u - P^1_{h_x} u\|_{L^2(Q)} \|u_h - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)},
\end{aligned}$$

and for the second term we have

$$\begin{aligned}
\langle \nabla_x (u - P^1_{h_x} Q^0_{h_t} u), \nabla_x \overline{v}_h\rangle_{L^2(Q)} &= \langle \nabla_x (u - Q^0_{h_t} u), \nabla_x \overline{v}_h\rangle_{L^2(Q)} \\
&= \langle \nabla_x (u - Q^0_{h_t} u), \nabla_x (\overline{v}_h - Q^0_{h_t} \overline{v}_h)\rangle_{L^2(Q)} \\
&\leq \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)} \|\nabla_x (\overline{v}_h - Q^0_{h_t} \overline{v}_h)\|_{L^2(Q)} \\
&\leq c\, h_x^{-1} \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)} \|\overline{v}_h - Q^0_{h_t} \overline{v}_h\|_{L^2(Q)} \\
&\leq c\, h_x^{-1}\, h_t \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)} \|\partial_t \overline{v}_h\|_{L^2(Q)} \\
&= c\, h_x^{-1}\, h_t \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)} \|u_h - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)}.
\end{aligned}$$

Hence we conclude

$$\|u_h - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)} \leq \|u - P^1_{h_x} u\|_{L^2(Q)} + c\, h_x^{-1}\, h_t \|\nabla_x (u - Q^0_{h_t} u)\|_{L^2(Q)}.$$

With

$$\|u - u_h\|_{L^2(Q)} \leq \|u - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)} + \|u_h - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)}$$

and

$$\begin{aligned}
\|u - P^1_{h_x} Q^0_{h_t} u\|_{L^2(Q)} &\leq \|u - Q^0_{h_t} u\|_{L^2(Q)} + \|Q^0_{h_t} (u - P^1_{h_x} u)\|_{L^2(Q)} \\
&\leq \|u - Q^0_{h_t} u\|_{L^2(Q)} + \|u - P^1_{h_x} u\|_{L^2(Q)},
\end{aligned}$$

the assertion follows. ■

Corollary 5.4 *Assume $u \in H^{2,1}(Q)$ such that $\nabla_x \partial_t u \in L^2(Q)$ is satisfied. Then there holds the error estimate*

$$\|u - u_h\|_{L^2(Q)} \leq c \left[h_x^2 \|u\|_{L^2(0,T;H^2(\Omega))} + h_t \|u\|_{H^1(0,T;L^2(\Omega))} + h_x^{-1}\, h_t^2 \|\nabla_x \partial_t u\|_{L^2(Q)} \right]. \quad (5.7)$$

In particular for $h_t \simeq h_x$ this gives

$$\|u - u_h\|_{L^2(Q)} \;\le\; c\, h_x \Big[h_x \, \|u\|_{L^2(0,T;H^2(\Omega))} + \|u\|_{H^1(0,T;L^2(\Omega))} + \|\nabla_x \partial_t u\|_{L^2(Q)} \Big], \tag{5.8}$$

while for $h_t \simeq h_x^2$ we obtain

$$\|u - u_h\|_{L^2(Q)} \;\le\; c\, h_x^2 \Big[\|u\|_{L^2(0,T;H^2(\Omega))} + \|u\|_{H^1(0,T;L^2(\Omega))} + h_x \, \|\nabla_x \partial_t u\|_{L^2(Q)} \Big]. \tag{5.9}$$

Even for a smooth solution u we therefore need to use the parabolic scaling $h_t \simeq h_x^2$ to ensure second order convergence in $L^2(Q)$ when using the adjoint formulation.

The need of a parabolic scaling to get higher order rates in $L^2(Q)$, also stems from the fact that for the adjoint formulation the ansatz space Y_h consists of only piecewise constant functions in time which do not give higher order convergence, even for smooth functions. This can be circumvented using a reconstruction operator in a post-processing step. To obtain a piecewise linear, globally continuous solution in time, we consider the following reconstruction operator $\mathcal{R}_{h_t} : W^0_{h_t} \to W^1_{h_t}$ where for each $u_{h_t} \in W^0_{h_t}$ given as

$$u_{h_t}(t) = \sum_{\ell=1}^{N} u_\ell \psi^0_\ell(t)$$

the reconstruction is defined as

$$(\mathcal{R}_{h_t} u_{h_t})(t) = \sum_{k=1}^{N} \bar{u}_k \psi^1_k(t), \tag{5.10}$$

where

$$\bar{u}_k = \frac{1}{2}\,(u_k + u_{k+1}) \quad \text{for } k = 1, \ldots, N-1, \quad \bar{u}_N = \frac{1}{2}\,(3u_N - u_{N-1}).$$

For ease of presentation, we assume that the temporal mesh is uniform. In the non-uniform case, define

$$\begin{aligned} \bar{u}_k &= \frac{h_{t,k}\, u_k + h_{t,k+1}\, u_{k+1}}{h_{t,k+1} + h_{t,k}} \quad \text{for } k = 1, \ldots, N-1, \\ \bar{u}_N &= \frac{(2h_{h,N} + h_{t,N-1})\, u_N - h_{t,N}\, u_{N-1}}{h_{t,N-1} + h_{t,N}}. \end{aligned}$$

By definition we set $(\mathcal{R}_{h_t} u_{h_t})(0) = 0$, i.e., $\bar{u}_0 = 0$. Similar reconstructions are well known for DG in time schemes, see, e.g., [18], for an excellent overview. The reconstruction operator satisfies the following properties.

Lemma 5.5 *For any $u_{h_t} \in W^0_{h_t}$ it holds that*

$$\|\mathcal{R}_{h_t} u_{h_t}\|_{L^2(t_{\ell-1},t_\ell)} \;\le\; c\, \|u_{h_t}\|_{L^2(\omega_\ell)} \quad \textit{for all } \ell = 1, \ldots, N, \tag{5.11}$$

where the element patch ω_ℓ is defined as

$$\omega_\ell = \begin{cases} (t_0, t_2), & \ell = 1, \\ (t_{\ell-2}, t_{\ell+1}), & \ell = 2, \ldots, N-1, \\ (t_{N-2}, t_N), & \ell = N. \end{cases}$$

Moreover, for any $u \in H^2(0,T)$ satisfying $u(0) = 0$ we have

$$\|u - \mathcal{R}_{h_t} Q^0_{h_t} u\|_{L^2(0,T)} \, \leq \, c\, h_t^2 \, |u|_{H^2(0,T)}. \tag{5.12}$$

Proof. For a piecewise constant function $u_{h_t} \in W^0_{h_t}$, given as

$$u_{h_t}(t) = \sum_{\ell=1}^{N} u_\ell \psi^0_\ell(t),$$

we have

$$\|u_{h_t}\|^2_{L^2(t_{\ell-1},t_\ell)} \, = \, h_t \, u_\ell^2, \quad \ell = 1, \ldots, N.$$

The reconstruction $\mathcal{R}_{h_t} u_{h_t}$ is a piecewise linear, globally continuous function,

$$(\mathcal{R}_{h_t} u_{h_t})(t) \, = \, \sum_{k=1}^{N} \bar{u}_k \psi^1_k(t).$$

On each temporal element $(t_{\ell-1}, t_\ell)$, we can compute

$$\begin{aligned} \|\mathcal{R}_{h_t} u_{h_t}\|^2_{L^2(t_{\ell-1},t_\ell)} \; &= \; \int_{t_{\ell-1}}^{t_\ell} \left[\frac{t_\ell - t}{t_\ell - t_{\ell-1}} \, \bar{u}_{\ell-1} + \frac{t - t_{\ell-1}}{t_\ell - t_{\ell-1}} \, \bar{u}_\ell \right]^2 dt \\ &= \; \frac{1}{3} \, h_t \left(\bar{u}^2_{\ell-1} + \bar{u}_{\ell-1} \bar{u}_\ell + \bar{u}^2_\ell \right) \, \leq \, \frac{1}{2} \, h_t \left(\bar{u}^2_{\ell-1} + \bar{u}^2_\ell \right). \end{aligned}$$

For all interior nodes, i.e., for $\ell = 1, \ldots, N-1$, we have

$$\bar{u}^2_\ell \, = \, \left(\frac{1}{2} \, (u_\ell + u_{\ell+1}) \right)^2 \, \leq \, \frac{1}{2} \left(u^2_\ell + u^2_{\ell+1} \right),$$

while for $\ell = N$ we get

$$\begin{aligned} \bar{u}^2_N \; &= \; \left(\frac{1}{2} \, (3u_N - u_{N-1}) \right)^2 \\ &= \; \frac{1}{4} \left(\begin{pmatrix} 9 & -3 \\ -3 & 1 \end{pmatrix} \begin{pmatrix} u_N \\ u_{N-1} \end{pmatrix}, \begin{pmatrix} u_N \\ u_{N-1} \end{pmatrix} \right) \, \leq \, \frac{5}{2} \left(u^2_N + u^2_{N-1} \right). \end{aligned}$$

Hence we obtain

$$\|\mathcal{R}_{h_t} u_{h_t}\|^2_{L^2(t_0,t_1)} \, \leq \, \frac{1}{2} \, h_t \, \bar{u}^2_1 \, \leq \, \frac{1}{4} \, h_t \left(u^2_1 + u^2_2 \right) \, = \, \frac{1}{4} \, \|u_{h_t}\|^2_{L^2(t_0,t_2)},$$

and for $\ell = 2, \dots, N-1$, we have

$$\|\mathcal{R}_{h_t} u_{h_t}\|^2_{L^2(t_{\ell-1},t_\ell)} \leq \frac{1}{2}\, h_t\left(\bar{u}^2_{\ell-1} + \bar{u}^2_\ell\right) \leq \frac{1}{4}\, h_t\left(u^2_{\ell-1} + 2u^2_\ell + u^2_{\ell+1}\right) \leq \frac{1}{2}\,\|u_{h_t}\|^2_{L^2(t_{\ell-2},t_{\ell+1})}.$$

It remains to consider $\ell = N$,

$$\|\mathcal{R}_{h_t} u_{h_t}\|^2_{L^2(t_{N-1},t_N)} \leq \frac{1}{2}\, h_t\left(\bar{u}^2_{N-1} + \bar{u}^2_N\right) \leq \frac{3}{2}\, h_t\left(u^2_{N-1} + u^2_N\right) \leq \frac{3}{2}\,\|u_{h_t}\|^2_{L^2(t_{N-2},t_N)}.$$

This concludes the proof of the stability estimate (5.11).

In order to prove (5.12) we consider an arbitrary linear function $q(t) = a + b\,t$ for which we compute

$$(Q^0_{h_t} q)(t) = \sum_{\ell=1}^N q_\ell \psi^0_\ell(t), \quad q_\ell \;=\; \frac{1}{h_t}\int_{t_{\ell-1}}^{t_\ell} q(t)\,dt \;=\; a + \frac{1}{2}\,b\,(t_\ell + t_{\ell-1}).$$

With this we further obtain

$$(\mathcal{R}_{h_t} Q^0_{h_t} q)(t) = \sum_{\ell=1}^N \bar{q}_\ell \psi^1_\ell(t),$$

with, for $\ell = 1, \dots, N-1$,

$$\bar{q}_\ell = \frac{1}{2}\,(q_\ell + q_{\ell+1}) = \frac{1}{2}\left(a + \frac{1}{2}\,b\,(t_\ell + t_{\ell-1}) + a + \frac{1}{2}\,b\,(t_{\ell+1} + t_\ell)\right) = a + b\,t_\ell = q(t_\ell),$$

where we have used $t_{\ell\pm1} = t_\ell \pm h_t$. Moreover, for $\ell = N$ we conclude

$$\begin{aligned}\bar{q}_N &= \frac{1}{2}\,(3q_N - q_{N-1}) = \frac{1}{2}\left(3\left(a + \frac{1}{2}\,b\,(t_N + t_{N-1})\right) - \left(a + \frac{1}{2}\,b\,(t_{N-1} + t_{N-2})\right)\right)\\ &= a + b\,t_N \;=\; q(t_N).\end{aligned}$$

Hence, on each interval $(t_{\ell-1}, t_\ell)$, $\ell = 2, \dots, N$, it holds that

$$(\mathcal{R}_{h_t} Q^0_{h_t} q)(t) = q(t)$$

for any affine linear function $q(t) = a + b\,t$, while on the first interval, (t_0, t_1), due to the homogeneous initial condition, we get

$$(\mathcal{R}_{h_t} Q^0_{h_t} q)(t) = q(t) \quad \text{for all } q(t) = b\,t.$$

Therefore we get for any $u \in H^2(\omega_\ell)$, using the stability estimate (5.11), that

$$\begin{aligned}\|u - \mathcal{R}_{h_t} Q^0_{h_t} u\|_{L^2(t_{\ell-1},t_\ell)} &= \|u - q + \mathcal{R}_{h_t} Q^0_{h_t}(q - u)\|_{L^2(t_{\ell-1},t_\ell)}\\ &\leq \|u - q\|_{L^2(t_{\ell-1},t_\ell)} + \|\mathcal{R}_{h_t} Q^0_{h_t}(q - u)\|_{L^2(t_{\ell-1},t_\ell)} \;\leq\; c\,\|u - q\|_{L^2(\omega_\ell)}.\end{aligned}$$

By standard approximation results, since q was arbitrary, we get for $\ell = 1$

$$\|u - \mathcal{R}_{h_t} Q^0_{h_t} u\|_{L^2(t_0,t_1)} \le c \inf_{q(t)=b\,t} \|u - q\|_{L^2(0,t_2)} \le c\,(2h_t)^2\, |u|_{H^2(\omega_\ell)},$$

and for $\ell = 2, \ldots, N$

$$\|u - \mathcal{R}_{h_t} Q^0_{h_t} u\|_{L^2(t_{\ell-1},t_\ell)} \le c \inf_{q(t)=a+b\,t} \|u - q\|_{L^2(\omega_\ell)} \le c\,(3h_t)^2\, |u|_{H^2(\omega_\ell)}.$$

Summing over all $\ell = 1, \ldots, N$ completes the proof. ∎

Theorem 5.6 *Let $u \in Y$ and $u_h \in Y_h$ be the unique solutions of (5.1) and (5.2), respectively. If $u \in H^2(0,T;L^2(\Omega)) \cap L^2(0,T;H^2(\Omega))$, $\nabla_x u \in H^2(0,T;L^2(\Omega))$ and $\partial_t \Delta_x u \in L^2(Q)$ are satisfied, then for $h_t \simeq h_x$ we have the error estimate*

$$\|u - \mathcal{R}_{h_t} u_h\|_{L^2(Q)} \le c(u)\, h_x^2,$$

where $c(u)$ is a constant depending on u.

Proof. We split the error

$$\|u - \mathcal{R}_{h_t} u_h\|_{L^2(Q)} \le \|u - \mathcal{R}_{h_t} Q^0_{h_t} P^1_{h_x} u\|_{L^2(Q)} + \|\mathcal{R}_{h_t} Q^0_{h_t} P^1_{h_x} u - \mathcal{R}_{h_t} u_h\|_{L^2(Q)}.$$

For the first term, using a Poincaré type inequality, the stability of $P^1_{h_x}$, as well as the error estimates (3.10) and (5.12), we get

$$\begin{aligned}
\|u - \mathcal{R}_{h_t} Q^0_{h_t} P^1_{h_x} u\|_{L^2(Q)} &\le \|u - P^1_{h_x} u\|_{L^2(Q)} + \|P^1_{h_x}(\mathcal{R}_{h_t} Q^0_{h_t} u - u)\|_{L^2(Q)} \\
&\le \|u - P^1_{h_x} u\|_{L^2(Q)} + c\,\|\nabla_x P^1_{h_x}(\mathcal{R}_{h_t} Q^0_{h_t} u - u)\|_{L^2(Q)} \\
&\le \|u - P^1_{h_x} u\|_{L^2(Q)} + c\,\|\nabla_x(\mathcal{R}_{h_t} Q^0_{h_t} u - u)\|_{L^2(Q)} \\
&\le c\left(h_x^2\, |u|_{L^2(0,T;H^2(\Omega))} + h_t^2\, |\nabla_x u|_{H^2(0,T;L^2(\Omega))}\right).
\end{aligned}$$

For the second term, using the stability estimate (5.11), we have that

$$\|\mathcal{R}_{h_t} Q^0_{h_t} P^1_{h_x} u - \mathcal{R}_{h_t} u_h\|_{L^2(Q)} \le c\,\|Q^0_{h_t} P^1_{h_x} u - u_h\|_{L^2(Q)}.$$

Now, we proceed similar as in the proof of Lemma 5.3. When using the Galerkin orthogonality

$$b_T(u, v_h) = b_T(u_h, v_h) \quad \text{for all}\, v_h \in X_{T,h},$$

we compute that

$$\begin{aligned}
b_T(Q^0_{h_t} P^1_{h_x} u - u_h, v_h) &= b_T(Q^0_{h_t} P^1_{h_x} u - u, v_h) \\
&= -\langle Q^0_{h_t} P^1_{h_x} u - u, \partial_t v_h\rangle_{L^2(Q)} + \langle \nabla_x(Q^0_{h_t} P^1_{h_x} u - u), \nabla_x v_h\rangle_{L^2(Q)} \\
&= -\langle Q^0_{h_t} P^1_{h_x} u - P^1_{h_x} u, \partial_t v_h\rangle_{L^2(Q)} - \langle P^1_{h_x} u - u, \partial_t v_h\rangle_{L^2(Q)} \\
&\qquad + \langle \nabla_x(Q^0_{h_t} u - u), \nabla_x v_h\rangle_{L^2(Q)} \\
&= -\langle P^1_{h_x} u - u, \partial_t v_h\rangle_{L^2(Q)} + \langle \nabla_x(Q^0_{h_t} u - u), \nabla_x(v_h - Q^0_{h_t} v_h)\rangle_{L^2(Q)}
\end{aligned}$$

In particular for

$$\overline{v}_h(x,t) := \int_t^T [Q^0_{h_t} P^1_{h_x} u(x,s) - u_h(x,s)]\, ds, \quad \overline{v}_h \in X_{T,h},$$

we get $-\partial_t \overline{v}_h = Q^0_{h_t} P^1_{h_x} u - u_h$, and

$$-\langle Q^0_{h_t} P^1_{h_x} u - u_h, \partial_t \overline{v}_h \rangle_{L^2(Q)} \;=\; \| Q^0_{h_t} P^1_{h_x} u - u_h \|^2_{L^2(Q)},$$

as well as

$$\begin{aligned}
\langle \nabla_x (Q^0_{h_t} P^1_{h_x} u - u_h), \nabla_x \overline{v}_h \rangle_{L^2(Q)} \;&=\; -\langle \nabla_x \partial_t \overline{v}_h, \nabla_x \overline{v}_h \rangle_{L^2(Q)} \\
&= -\frac{1}{2} \int_0^T \frac{d}{dt} \| \nabla_x \overline{v}_h(t) \|^2_{L^2(\Omega)}\, dt \;=\; \frac{1}{2} \| \nabla_x \overline{v}_h(0) \|^2_{L^2(\Omega)} \;\geq\; 0.
\end{aligned}$$

Hence, we get

$$\begin{aligned}
&\| Q^0_{h_t} P^1_{h_x} u - u_h \|^2_{L^2(Q)} \\
&\quad\leq\; -\langle Q^0_{h_t} P^1_{h_x} u - u_h, \partial_t \overline{v}_h \rangle_{L^2(Q)} + \langle \nabla_x (Q^0_{h_t} P^1_{h_x} u - u_h), \nabla_x \overline{v}_h \rangle_{L^2(Q)} \\
&\quad=\; b_T(Q^0_{h_t} P^1_{h_x} u - u_h, \overline{v}_h) \\
&\quad=\; -\langle P^1_{h_x} u - u, \partial_t \overline{v}_h \rangle_{L^2(Q)} + \langle \nabla_x (Q^0_{h_t} u - u), \nabla_x (\overline{v}_h - Q^0_{h_t} \overline{v}_h) \rangle_{L^2(Q)}.
\end{aligned}$$

Now, using the Cauchy–Schwarz inequality and (3.10), the first term is estimated by

$$\begin{aligned}
-\langle P^1_{h_x} u - u, \partial_t \overline{v}_h \rangle_{L^2(Q)} \;&\leq\; \| P^1_{h_x} u - u \|_{L^2(Q)} \| \partial_t \overline{v}_h \|_{L^2(Q)} \\
&\leq\; c\, h_x^2\, |u|_{L^2(0,T;H^2(\Omega))} \| \partial_t \overline{v}_h \|_{L^2(Q)},
\end{aligned}$$

while for the second term, using integration by parts and (3.14), this gives

$$\begin{aligned}
\langle \nabla_x (Q^0_{h_t} u - u), \nabla_x (\overline{v}_h - Q^0_{h_t} \overline{v}_h) \rangle_{L^2(Q)} \;&=\; \langle -\Delta_x (Q^0_{h_t} u - u), \overline{v}_h - Q^0_{h_t} \overline{v}_h \rangle_{L^2(Q)} \\
\leq\; \| \Delta_x (Q^0_{h_t} u - u) \|_{L^2(Q)} \| \overline{v}_h - Q^0_{h_t} \overline{v}_h \|_{L^2(Q)} \;&\leq\; c\, h_t^2\, \| \Delta_x \partial_t u \|_{L^2(Q)} \| \partial_t \overline{v}_h \|_{L^2(Q)}.
\end{aligned}$$

With $h_x \simeq h_t$ and $\partial_t \overline{v}_h = Q^0_{h_t} P^1_{h_x} u - u_h$, we finally obtain

$$\| Q^0_{h_t} P^1_{h_x} u - u_h \|_{L^2(Q)} \;\leq\; c\, h_x^2 \Big(\|u\|_{L^2(0,T;H^2(\Omega))} + \|u\|_{H^1(0,T;H^2(\Omega))} \Big),$$

and the assertion follows. ■

It remains to consider the case of less regular initial data:

Corollary 5.7 *Let $u \in Y$ and $u_h \in Y_h$ be the unique solutions of the variational formulations* (5.1) *and* (5.2), *respectively. Assume $f \equiv 0$, and $u_0 \in \widetilde{H}^s(\Omega) := [L^2(\Omega), H^1_0(\Omega)]_{|s}$ for* *some $s \in [0,1]$. Then, $u \in H^{1+s,(1+s)/2}(Q) \cap H^{s/2}(0,T;H^1_0(\Omega))$. The error estimate (5.6) then gives*

$$\begin{aligned}\|u-u_h\|_{L^2(Q)} \;&\leq\; c\Big[h_x^{1+s}\,\|u\|_{L^2(0,T;H^{1+s}(\Omega))}+h_t^{(1+s)/2}\,\|u\|_{H^{(1+s)/2}(0,T;L^2(\Omega))}\\ &\qquad +h_x^{-1}\,h_t\,h_t^{s/2}\,\|u\|_{H^{s/2}(0,T;H^1_0(\Omega))}\Big],\end{aligned}$$

and in particular for $h_t \simeq h_x^2$ we obtain

$$\begin{aligned}&\|u-u_h\|_{L^2(Q)}\\ &\quad\leq\; c\,h_x^{1+s}\Big[\|u\|_{L^2(0,T;H^{1+s}(\Omega))}+\|u\|_{H^{(1+s)/2}(0,T;L^2(\Omega))}+\|u\|_{H^{s/2}(0,T;H^1_0(\Omega))}\Big].\end{aligned}$$

Note that for a discontinuous but piecewise smooth initial datum we have $u_0 \in \widetilde{H}^s(\Omega)$, $s<\frac{1}{2}$.

It remains to take a closer look on the discrete variational formulation (5.2). When writing

$$u_h(x,t) \;=\; \sum_{i=1}^{N_t}\sum_{k=1}^{M_x} u_k^i\,\psi_i^0(t)\,\varphi_k(x) \;=\; \sum_{k=1}^{M_x} u_k(t)\,\varphi_k(x),$$

and using as test function $v_h(x,t)=\psi_j^1(t)\varphi_\ell(x)$, $j=1,\ldots,N_t-1$, $\ell=1,\ldots,M_x$, (5.2) is equivalent to, recall $\psi_j^1(0)=0$ for $j=1,\ldots,N_t-1$,

$$\begin{aligned}-\sum_{k=1}^{M_x}\int_{t_{j-1}}^{t_{j+1}} u_k(t)\,\partial_t\psi_j^1(t)\,dt\int_\Omega \varphi_k(x)\varphi_\ell(x)dx&\\ +\sum_{k=1}^{M_x}\int_{t_{j-1}}^{t_{j+1}} u_k(t)\psi_j^1(t)\,dt\int_\Omega \nabla_x\varphi_k(x)\cdot\nabla_x\varphi_\ell(x)\,dx&\\ =\int_{t_{j-1}}^{t_{j+1}}\int_\Omega f(x,t)\varphi_\ell(x)\,dx\,\psi_j^1(t)\,dt&,\end{aligned}$$

which we can write as Crank–Nicolson scheme

$$M_h(\underline{u}^{j+1}-\underline{u}^j)+\frac{1}{2}\,h_t\,K_h(\underline{u}^{j+1}+\underline{u}^j)\;=\;\underline{f}^j, \tag{5.13}$$

with the spatial mass and stiffness matrices M_h and K_h. Note that the coefficient vector $\underline{u}^j$ describes the solution which is constant in the time interval (t_j,t_{j+1}). For the remaining test functions $v_h(x,t)=\psi_0^1(t)\varphi_\ell(x)$, $\ell=1,\ldots,M_x$, we have

$$\begin{aligned}-\sum_{k=1}^{M_x}\int_{t_0}^{t_1} u_k(t)\,\partial_t\psi_0^1(t)\,dt\int_\Omega \varphi_k(x)\varphi_\ell(x)dx&\\ +\sum_{k=1}^{M_x}\int_{t_0}^{t_1} u_k(t)\psi_0^1(t)\,dt\int_\Omega \nabla_x\varphi_k(x)\cdot\nabla_x\varphi_\ell(x)\,dx&\\ =\int_{t_0}^{t_1}\int_\Omega f(x,t)\varphi_\ell(x)\,dx\,\psi_0^1(t)\,dt+\int_\Omega u_0(x)\varphi_\ell(x)\,dx&,\end{aligned}$$

i.e., we obtain the implicit Euler scheme

$$M_h \underline{u}^1 + \frac{1}{2}\, h_t\, K_h \underline{u}^1 = \underline{f}^0 + \underline{u}^0. \tag{5.14}$$

In particular, the adjoint formulation corresponds to a time stepping scheme, where for the first step implicit Euler is used with step size $h_t/2$, and then Crank–Nicolson is applied with step size h_t. Such a scheme was already proposed by Rannacher [26] known as *Rannacher smoothing*, to regularize the initial datum u_0 and get a more stable numerical approximation. Indeed, one could also see the first implicit Euler step as a smoothing projection $\Pi^1_{h_x} : L^2(\Omega) \to V_{h_x}$ given as

$$\langle \Pi^1_{h_x} u_0, v_{h_x} \rangle_{L^2(\Omega)} + \frac{h_t}{2} \langle \nabla_x \Pi^1_{h_x} u_0, \nabla_x v_{h_x} \rangle_{L^2(\Omega)} \;=\; \langle u_0, v_{h_x} \rangle_{L^2(\Omega)}, \quad \text{for all } v_{h_x} \in V_{h_x}. \tag{5.15}$$

Then the adjoint formulation corresponds to a perturbed primal formulation in which the initial datum u_0 is projected by $\Pi^1_{h_x}$ rather than by $Q^1_{h_x}$. Since the projection $\Pi^1_{h_x}$ regularizes the initial datum, the error analysis of the primal formulation for smooth data can be applied. To obtain the convergence rate of this scheme, it remains to estimate the projection error of the initial condition.

Lemma 5.8 *For $u_0 \in L^2(\Omega)$ there holds*

$$\|\Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; \|u_0\|_{L^2(\Omega)}, \quad \textit{and} \quad \|\nabla_x \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; \sqrt{2}\, h_t^{-1/2}\, \|u_0\|_{L^2(\Omega)}, \tag{5.16}$$

as well as

$$\|u_0 - \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; \|u_0\|_{L^2(\Omega)}. \tag{5.17}$$

Moreover, if $u_0 \in H^1_0(\Omega)$, then

$$\|\nabla_x \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; c \left(1 + h_x^2\, h_t^{-1}\right)^{1/2} \|\nabla_x u_0\|_{L^2(\Omega)}, \tag{5.18}$$

$$\|u_0 - \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; c \left(h_t + h_x^2\right)^{1/2} \|\nabla_x u_0\|_{L^2(\Omega)}, \tag{5.19}$$

and

$$\|\nabla_x (u_0 - \Pi^1_{h_x} u_0)\|_{L^2(\Omega)} \;\le\; c \left(1 + h_x^2\, h_t^{-1}\right)^{1/2} \|\nabla_x u_0\|_{L^2(\Omega)}. \tag{5.20}$$

Moreover, if $u_0 \in H^2(\Omega) \cap H^1_0(\Omega)$ is satisfied, then

$$\|u_0 - \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \;\le\; c \left(h_t + h_x^2\right) |u_0|_{H^2(\Omega)}, \tag{5.21}$$

and

$$\|\nabla_x (u_0 - \Pi^1_{h_x} u_0)\|_{L^2(\Omega)} \;\le\; c \left(h_t + h_x^4\, h_t^{-1} + h_x^2\right)^{1/2} |u_0|_{H^2(\Omega)}. \tag{5.22}$$

Proof. When testing (5.15) with $v_{h_x} = \Pi^1_{h_x} u_0 \in V_{h_x}$ this gives

$$\|\Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \;=\; \langle u_0, \Pi^1_{h_x} u_0\rangle_{L^2(\Omega)} \;\le\; \|u_0\|_{L^2(\Omega)} \|\Pi^1_{h_x} u_0\|_{L^2(\Omega)},$$

from which (5.16) follows. Moreover, we compute, using (5.15) for $v_h = \Pi^1_{h_x} u_0$,

$$\begin{aligned}
&\|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \\
&\quad= \|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\langle \nabla_x \Pi^1_{h_x} u_0, \nabla_x \Pi^1_{h_x} u_0\rangle_{L^2(\Omega)} \\
&\quad= \|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \langle u_0 - \Pi^1_{h_x} u_0, \Pi^1_{h_x} u_0\rangle_{L^2(\Omega)} \\
&\quad= \langle u_0 - \Pi^1_{h_x} u_0, u_0\rangle_{L^2(\Omega)} \;\le\; \|u_0 - \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \|u_0\|_{L^2(\Omega)},
\end{aligned}$$

from which (5.17) follows. For $u_0 \in H^1_0(\Omega)$ we can consider the H^1_0 projection $P^1_{h_x} u_0 \in V_{h_x}$, and using the same computations as above as well as Hölder's inequality we conclude

$$\begin{aligned}
\|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \;&=\; \langle u_0 - \Pi^1_{h_x} u_0, u_0\rangle_{L^2(\Omega)} \\
&= \langle u_0 - \Pi^1_{h_x} u_0, u_0 - P^1_{h_x} u_0\rangle_{L^2(\Omega)} + \langle u_0 - \Pi^1_{h_x} u_0, P^1_{h_x} u_0\rangle_{L^2(\Omega)} \\
&= \langle u_0 - \Pi^1_{h_x} u_0, u_0 - P^1_{h_x} u_0\rangle_{L^2(\Omega)} + \frac{h_t}{2}\,\langle \nabla_x \Pi^1_{h_x} u_0, \nabla_x P^1_{h_x} u_0\rangle_{L^2(\Omega)} \\
&\le \|u_0 - \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \|u_0 - P^1_{h_x} u_0\|_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|_{L^2(\Omega)} \|\nabla_x P^1_{h_x} u_0\|_{L^2(\Omega)} \\
&\le \left(\|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \right)^{1/2} \\
&\qquad \cdot \left(\|u_0 - P^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x P^1_{h_x} u_0\|^2_{L^2(\Omega)} \right)^{1/2},
\end{aligned}$$

i.e.,

$$\|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \;\le\; \|u_0 - P^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x P^1_{h_x} u_0\|^2_{L^2(\Omega)}.$$

With the error estimate (3.10) and the stability of $P^1_{h_x} : H^1_0(\Omega) \to V_{h_x} \subset H^1_0(\Omega)$ we further obtain

$$\|u_0 - P^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} \;\le\; c\left[h_x^2 + h_t\right] \|\nabla_x u_0\|^2_{L^2(\Omega)},$$

which gives (5.18) and (5.19). Moreover, (5.15) is equivalent to

$$\frac{h_t}{2}\,\langle \nabla_x (\Pi^1_{h_x} u_0 - P^1_{h_x} u_0), \nabla_x v_h\rangle_{L^2(\Omega)} = \langle u_0 - \Pi^1_{h_x} u_0, v_h\rangle_{L^2(\Omega)} - \frac{h_t}{2}\,\langle \nabla_x P^1_{h_x} u_0, \nabla_x v_h\rangle_{L^2(\Omega)}$$

for all $v_h \in V_{h_x}$. In particular for $v_h = \Pi^1_{h_x} u_0 - P^1_{h_x} u_0$ this gives

$$
\begin{aligned}
&\frac{h_t}{2}\,\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\qquad\qquad = \langle u_0 - \Pi^1_{h_x}u_0, \Pi^1_{h_x}u_0 - P^1_{h_x}u_0\rangle_{L^2(\Omega)} \\
&\qquad\qquad\qquad + \frac{h_t}{2}\,\langle \nabla_x P^1_{h_x}u_0, \nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\rangle_{L^2(\Omega)} \\
&\qquad\qquad = \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\|\Pi^1_{h_x}u_0 - P^1_{h_x}u_0\|_{L^2(\Omega)} \\
&\qquad\qquad\qquad + \frac{h_t}{2}\,\|\nabla_x P^1_{h_x}u_0\|_{L^2(\Omega)}\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)} \\
&\qquad\qquad \le \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\Big[\|\Pi^1_{h_x}u_0 - u_0\|_{L^2(\Omega)} + \|u_0 - P^1_{h_x}u_0\|_{L^2(\Omega)}\Big] \\
&\qquad\qquad\qquad + \frac{h_t}{2}\,\|\nabla_x P^1_{h_x}u_0\|_{L^2(\Omega)}\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)} \\
&\qquad\qquad \le c\left(h_t + h_x^2\right)^{1/2}\|\nabla_x u_0\|_{L^2(\Omega)} \\
&\qquad\qquad\qquad\qquad \cdot\Big[c\left(h_t + h_x^2\right)^{1/2}\|\nabla_x u_0\|_{L^2(\Omega)} + c\,h_x\,\|\nabla_x u_0\|_{L^2(\Omega)}\Big] \\
&\qquad\qquad\qquad + \frac{h_t}{2}\,\|\nabla_x u_0\|_{L^2(\Omega)}\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)} \\
&\qquad\qquad \le c\left(h_t + h_x^2\right)\|\nabla_x u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x u_0\|_{L^2(\Omega)}\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)},
\end{aligned}
\tag{5.23}
$$

when using the error estimates (5.19) and (3.10), and the stability estimate (3.8). Hence we have shown

$$
\begin{aligned}
&\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad \le 2\,c\left(1 + h_x^2\,h_t^{-1}\right)\|\nabla_x u_0\|^2_{L^2(\Omega)} + \|\nabla_x u_0\|_{L^2(\Omega)}\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)},
\end{aligned}
$$

from which

$$\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|_{L^2(\Omega)} \le c\left(1 + h_x^2\,h_t^{-1}\right)^{1/2}\|\nabla_x u_0\|_{L^2(\Omega)}$$

follows. With

$$\|\nabla_x(u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)} \le \|\nabla_x(u_0 - P^1_{h_x}u_0)\|_{L^2(\Omega)} + \|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|_{L^2(\Omega)}$$

and using (3.9) for $s = 1$ we conclude (5.20).

It remains to consider the case $u_0 \in H^2(\Omega) \cap H^1_0(\Omega)$. Note that (5.23) can be rewritten as

$$
\begin{aligned}
&\|u_0 - \Pi^1_{h_x}u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad = \langle u_0 - \Pi^1_{h_x}u_0, u_0 - P^1_{h_x}u_0\rangle_{L^2(\Omega)} + \frac{h_t}{2}\,\langle \nabla_x P^1_{h_x}u_0, \nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\rangle_{L^2(\Omega)} \\
&\quad = \langle u_0 - \Pi^1_{h_x}u_0, u_0 - P^1_{h_x}u_0\rangle_{L^2(\Omega)} + \frac{h_t}{2}\,\langle \nabla_x u_0, \nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\rangle_{L^2(\Omega)},
\end{aligned}
$$

using the definition (3.7) of $P^1_{h_x}$. Using integration by parts, we further conclude

$$\begin{aligned}
&\|u_0 - \Pi^1_{h_x} u_0\|^2_{L^2(\Omega)} + \frac{h_t}{2}\,\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad = \langle u_0 - \Pi^1_{h_x}u_0, u_0 - P^1_{h_x}u_0\rangle_{L^2(\Omega)} + \frac{h_t}{2}\,\langle -\Delta_x u_0, P^1_{h_x}u_0 - \Pi^1_{h_x}u_0\rangle_{L^2(\Omega)} \\
&\quad \le \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\|u_0 - P^1_{h_x}u_0\|_{L^2(\Omega)} \\
&\qquad\qquad + \frac{h_t}{2}\,\|\Delta_x u_0\|_{L^2(\Omega)}\|P^1_{h_x}u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)} \\
&\quad \le \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\|u_0 - P^1_{h_x}u_0\|_{L^2(\Omega)} \\
&\qquad\qquad + \frac{h_t}{2}\,\|\Delta_x u_0\|_{L^2(\Omega)}\Big[\|P^1_{h_x}u_0 - u_0\|_{L^2(\Omega)} + \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\Big] \\
&\quad \le c\,h_x^2\,\|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}|u_0|_{H^2(\Omega)} \\
&\qquad\qquad + \frac{h_t}{2}\,|u_0|_{H^2(\Omega)}\Big[c\,h_x^2\,|u_0|_{H^2(\Omega)} + \|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}\Big],
\end{aligned}$$

where we have used the error estimate (3.10) for $s = 2$. Hence we have shown

$$\|u_0 - \Pi^1_{h_x}u_0\|^2_{L^2(\Omega)} \le c\left(h_x^2 + h_t\right)|u_0|_{H^2(\Omega)}\|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)} + c\,h_x^2\,h_t\,|u_0|^2_{H^2(\Omega)},$$

from which

$$\|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)} \le c\left(h_x^2 + h_t\right)|u_0|_{H^2(\Omega)}$$

follows, i.e., (5.21). With this we further conclude

$$\begin{aligned}
&\|\nabla_x(\Pi^1_{h_x}u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad \le c\left(1 + h_x^2\,h_t^{-1}\right)\|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)}|u_0|_{H^2(\Omega)} + c\,h_x^2\,|u_0|^2_{H^2(\Omega)} \\
&\quad \le c\left[\left(1 + h_x^2\,h_t^{-1}\right)\left(h_x^2 + h_t\right) + h_x^2\right]|u_0|^2_{H^2(\Omega)}.
\end{aligned}$$

With the triangle inequality

$$\begin{aligned}
&\|\nabla_x(u_0 - \Pi^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad \le 2\,\|\nabla_x(u_0 - P^1_{h_x}u_0)\|^2_{L^2(\Omega)} + 2\,\|\nabla_x(P^1_{h_x}u_0 - \Pi^1_{h_x}u_0)\|^2_{L^2(\Omega)} \\
&\quad \le c\left[\left(1 + h_x^2\,h_t^{-1}\right)\left(h_x^2 + h_t\right) + h_x^2\right]|u_0|^2_{H^2(\Omega)}
\end{aligned}$$

we finally conclude (5.22). ■

When considering the error estimates (5.17) and (5.19) we can use a space interpolation argument to conclude the following result:

Theorem 5.9 *Assume* $u_0 \in \widetilde{H}^s(\Omega) := [L^2(\Omega), H^1_0(\Omega)]_{|s}$ *for some* $s \in [0,1]$. *Then there holds the error estimate*

$$\|u_0 - \Pi^1_{h_x}u_0\|_{L^2(\Omega)} \le c\left(h_x^2 + h_t\right)^{s/2}\|u_0\|_{\widetilde{H}^s(\Omega)}. \tag{5.24}$$

6 Numerical results

As a numerical example we consider the heat equation (1.1) in the one-dimensional spatial domain $\Omega = (0,1)$ and $T = 1$. The space-time finite element discretization of the primal variational formulation (2.6) is done by using the ansatz space $X_{0,h} = W^1_{h_t} \otimes V_{h_x}$ and the test space $Y_h = W^0_{h_t} \otimes V_{h_x}$, while for the adjoint formulation (5.2) we use Y_h as ansatz space, and $X_{T,h} = \overline{W}^1_{h_t} \otimes V_{h_x}$ as test space. First, we consider the smooth solution

$$u(x,t) = \cos(\pi t)\sin(\pi x) \tag{6.1}$$

where the given data f and u_0 are computed from u. The numerical results for both the primal and the adjoint formulation using $h_t = h_x$ are given in Table 1, where we observe first order convergence in $Y = L^2(0,T;H^1_0(\Omega))$ in both cases, as predicted by Theorem 4.6 and Theorem 5.2, respectively. However, we only observe second order convergence in $L^2(Q)$ for the primal formulation as explained by Lemma 4.5, while the error for the adjoint approach converges linearly, see Corollary 5.4. To obtain second order convergence in $L^2(Q)$ also for the adjoint formulation, we need to postprocess the solution, see Theorem 5.6, or use parabolic scaling, see Table 2, and Table 3.

N_x	N_t	$\|u-u_h\|_{L^2(Q)}$	eoc	$\|u-u_h\|_Y$	eoc
		primal formulation			
4	4	$4.137 \cdot 10^{-2}$		$3.597 \cdot 10^{-1}$	
8	8	$1.027 \cdot 10^{-2}$	2.01	$1.784 \cdot 10^{-1}$	1.01
16	16	$2.562 \cdot 10^{-3}$	2.00	$8.907 \cdot 10^{-2}$	1.00
32	32	$6.403 \cdot 10^{-4}$	2.00	$4.452 \cdot 10^{-2}$	1.00
64	64	$1.601 \cdot 10^{-4}$	2.00	$2.226 \cdot 10^{-2}$	1.00
128	128	$4.001 \cdot 10^{-5}$	2.00	$1.113 \cdot 10^{-2}$	1.00
256	256	$1.000 \cdot 10^{-5}$	2.00	$5.565 \cdot 10^{-3}$	1.00
		adjoint formulation			
4	4	$1.129 \cdot 10^{-1}$		$4.988 \cdot 10^{-1}$	
8	8	$5.661 \cdot 10^{-2}$	1.00	$2.512 \cdot 10^{-1}$	0.99
16	16	$2.833 \cdot 10^{-2}$	1.00	$1.258 \cdot 10^{-1}$	1.00
32	32	$1.417 \cdot 10^{-2}$	1.00	$6.295 \cdot 10^{-2}$	1.00
64	64	$7.085 \cdot 10^{-3}$	1.00	$3.148 \cdot 10^{-2}$	1.00
128	128	$3.543 \cdot 10^{-3}$	1.00	$1.574 \cdot 10^{-2}$	1.00
256	256	$1.771 \cdot 10^{-3}$	1.00	$7.870 \cdot 10^{-3}$	1.00

Table 1: Convergence results for the primal and adjoint formulations in the case of the smooth solution (6.1), $h_t = h_x$.

As a second example, we consider, similar to [36], the solution

$$u(x,t) = \sum_{\ell=1}^{\infty} \frac{4}{\ell\pi} \sin\left(\frac{\ell\pi}{2}\right) \sin\left(\frac{\ell\pi}{4}\right) e^{-\ell^2\pi^2 t} \sin(\ell\pi x). \tag{6.2}$$

adjoint formulation					
N_x	N_t	$\|u-u_h\|_{L^2(Q)}$	eoc	$\|u-u_h\|_Y$	eoc
4	16	$5.110 \cdot 10^{-2}$		$4.784 \cdot 10^{-1}$	
8	64	$1.054 \cdot 10^{-2}$	2.28	$2.044 \cdot 10^{-1}$	1.23
16	256	$2.452 \cdot 10^{-3}$	2.10	$9.509 \cdot 10^{-2}$	1.10
32	1024	$5.944 \cdot 10^{-4}$	2.04	$4.597 \cdot 10^{-2}$	1.05
64	4096	$1.465 \cdot 10^{-4}$	2.02	$2.261 \cdot 10^{-2}$	1.02
128	16384	$3.638 \cdot 10^{-5}$	2.01	$1.122 \cdot 10^{-2}$	1.01

Table 2: Convergence results for the adjoint formulation in the case of the smooth solution (6.1) with parabolic scaling, $h_t = h_x^2$.

adjoint formulation					
N_x	N_t	$\|u-\mathcal{R}_{h_t}u_h\|_{L^2(Q)}$	eoc	$\|u-\mathcal{R}_{h_t}u_h\|_Y$	eoc
4	4	$6.186 \cdot 10^{-2}$		$3.847 \cdot 10^{-1}$	
8	8	$1.779 \cdot 10^{-2}$	1.798	$1.822 \cdot 10^{-1}$	1.078
16	16	$4.705 \cdot 10^{-3}$	1.918	$8.957 \cdot 10^{-2}$	1.024
32	32	$1.205 \cdot 10^{-3}$	1.965	$4.459 \cdot 10^{-2}$	1.006
64	64	$3.047 \cdot 10^{-4}$	1.984	$2.227 \cdot 10^{-2}$	1.002
128	128	$7.656 \cdot 10^{-5}$	1.992	$1.113 \cdot 10^{-2}$	1.000
256	256	$1.919 \cdot 10^{-5}$	1.996	$5.565 \cdot 10^{-3}$	1.000

Table 3: Convergence results for the adjoint formulation with reconstruction in the case of the smooth solution (6.1) and uniform scaling, $h_t = h_x$.

which is a solution of the homogeneous heat equation (1.1) with $f \equiv 0$, and with the initial datum

$$u_0(x) = \begin{cases} 1, & \text{if } x \in (0.25, 0.75), \\ 0, & \text{else.} \end{cases}$$

The numerical results for both the primal and adjoint formulations are given in Table 4. In the case of orthotropic scaling, $h_t = h_x$, we observe divergence of the primal formulation in Y, as can be explained by (4.12), where $c_{S,h} \simeq h_x$, and using the best approximation in X. For the adjoint formulation, though, we see a rate of $1/4$, as predicted by Theorem 5.9 for all $s < 1/2$. The rates for the error in $L^2(Q)$ are not yet explained by the theory presented. When using parabolic scaling, $h_t = h_x^2$, in Table 5 in both cases we obtain comparable results with orders of convergence which are due to the reduced regularity of the solution as explained by (4.12) and (5.4) for the primal and adjoint formulation, respectively, using $c_{S,h} \simeq 1$, and the best approximation in the corresponding norms.
Even though the convergence behavior is similar, the adjoint approach does not overshoot at the discontinuities of the initial data. This behavior is exemplified in Figure 1 for the primal and adjoint approach for $N_x = N_t = 32$, see also [36] for a more detailed discussion

N_x	N_t	$\|u-u_h\|_{L^2(Q)}$	eoc	$\|u-u_h\|_Y$	eoc
		primal formulation			
4	4	$8.878 \cdot 10^{-2}$		$8.377 \cdot 10^{-1}$	
8	8	$7.222 \cdot 10^{-2}$	0.30	$1.115 \cdot 10^{0}$	-0.41
16	16	$5.545 \cdot 10^{-2}$	0.38	$1.599 \cdot 10^{0}$	-0.52
32	32	$4.091 \cdot 10^{-2}$	0.44	$2.269 \cdot 10^{0}$	-0.50
64	64	$2.959 \cdot 10^{-2}$	0.47	$3.183 \cdot 10^{0}$	-0.49
		adjoint formulation			
4	4	$8.944 \cdot 10^{-2}$		$3.498 \cdot 10^{-1}$	
8	8	$5.273 \cdot 10^{-2}$	0.76	$2.753 \cdot 10^{-1}$	0.35
16	16	$3.073 \cdot 10^{-2}$	0.78	$2.356 \cdot 10^{-1}$	0.22
32	32	$1.832 \cdot 10^{-2}$	0.75	$2.025 \cdot 10^{-1}$	0.22
64	64	$1.091 \cdot 10^{-2}$	0.75	$1.725 \cdot 10^{-1}$	0.23

Table 4: Convergence results for the primal and adjoint formulations for the singular solution (6.2) with discontinuous initial data, $h_t = h_x$.

N_x	N_t	$\|u-u_h\|_{L^2(Q)}$	eoc	$\|u-u_h\|_Y$	eoc
		primal formulation			
4	16	$2.265 \cdot 10^{-2}$		$3.091 \cdot 10^{-1}$	
8	64	$7.467 \cdot 10^{-3}$	1.60	$1.979 \cdot 10^{-1}$	0.64
16	256	$2.642 \cdot 10^{-3}$	1.50	$1.397 \cdot 10^{-1}$	0.50
32	1024	$9.314 \cdot 10^{-4}$	1.50	$9.854 \cdot 10^{-2}$	0.50
64	4096	$3.264 \cdot 10^{-4}$	1.51	$6.920 \cdot 10^{-2}$	0.51
		adjoint formulation			
4	16	$3.073 \cdot 10^{-2}$		$2.435 \cdot 10^{-1}$	
8	64	$1.088 \cdot 10^{-2}$	1.50	$1.726 \cdot 10^{-1}$	0.50
16	256	$3.848 \cdot 10^{-3}$	1.50	$1.221 \cdot 10^{-1}$	0.50
32	1024	$1.360 \cdot 10^{-3}$	1.50	$8.629 \cdot 10^{-2}$	0.50
64	4096	$4.807 \cdot 10^{-4}$	1.50	$6.090 \cdot 10^{-2}$	0.50

Table 5: Convergence results for the primal and adjoint formulations for the singular solution (6.2) with discontinuous initial data and parabolic scaling, $h_t = h_x^2$.

of the Crank–Nicolson oscillations.

Although we have presented almost all error estimates in the case of lowest order finite element spaces only, these results can be generalized to higher order polynomial ansatz spaces. To ensure optimal convergence, a related higher regularity of the solution is required, excluding discontinuous initial data. For the smooth solution as given in (6.1) we provide some numerical results, in which we first consider second order finite elements in space, and second order finite elements in time as ansatz functions, but piecewise linear

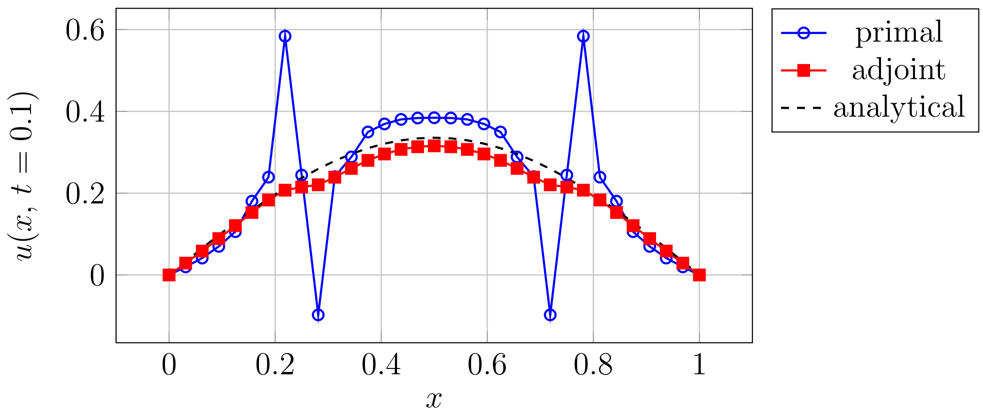

Figure 1: Comparison of the primal and adjoint approach at $t = 0.1$.

ones for testing. In the adjoint formulation we switch ansatz and test spaces accordingly. The numerical results as given in Table 6 indicate optimal orders of convergence, as expected. Finally, in Table 7 we provide related results for cubic finite elements in space and time, and second order test functions in time for the primal formulation. For the adjoint formulation, second order functions in time are used as ansatz, while third order finite elements are used for testing. Again we observe optimal orders of convergence, as expected.

N_x	N_t	$\|u - u_h\|_{L^2(Q)}$	eoc	$\|u - u_h\|_Y$	eoc
		primal formulation			
2	2	$5.78 \cdot 10^{-2}$		$1.12 \cdot 10^{-1}$	
4	4	$1.71 \cdot 10^{-2}$	1.76	$2.02 \cdot 10^{-1}$	-0.85
8	8	$2.49 \cdot 10^{-3}$	2.78	$5.13 \cdot 10^{-2}$	1.98
16	16	$3.25 \cdot 10^{-4}$	2.94	$1.28 \cdot 10^{-2}$	2.00
32	32	$4.10 \cdot 10^{-5}$	2.98	$3.20 \cdot 10^{-3}$	2.00
64	64	$5.15 \cdot 10^{-6}$	2.99	$7.99 \cdot 10^{-4}$	2.00
		adjoint formulation			
2	2	$4.64 \cdot 10^{-2}$		$2.05 \cdot 10^{-1}$	
4	4	$1.20 \cdot 10^{-2}$	1.95	$5.17 \cdot 10^{-2}$	1.98
8	8	$2.92 \cdot 10^{-3}$	2.04	$1.28 \cdot 10^{-2}$	2.01
16	16	$7.22 \cdot 10^{-4}$	2.02	$3.20 \cdot 10^{-3}$	2.00
32	32	$1.80 \cdot 10^{-4}$	2.01	$7.98 \cdot 10^{-4}$	2.00
64	64	$4.49 \cdot 10^{-5}$	2.00	$2.00 \cdot 10^{-4}$	2.00

Table 6: Convergence results for the primal and adjoint formulations using quadratic/linear finite elements in time, and quadratic/quadratic finite elements in space in the case of the smooth solution (6.1), $h_t = h_x$.

N_x	N_t	$\|u-u_h\|_{L^2(Q)}$	eoc	$\|u-u_h\|_Y$	eoc
primal formulation					
2	2	$4.48 \cdot 10^{-2}$		$7.76 \cdot 10^{-2}$	
4	4	$2.20 \cdot 10^{-3}$	4.35	$6.86 \cdot 10^{-3}$	3.50
8	8	$1.31 \cdot 10^{-4}$	4.07	$7.25 \cdot 10^{-4}$	3.24
16	16	$8.01 \cdot 10^{-6}$	4.03	$8.39 \cdot 10^{-5}$	3.11
32	32	$4.98 \cdot 10^{-7}$	4.01	$1.02 \cdot 10^{-5}$	3.03
64	64	$3.11 \cdot 10^{-8}$	4.00	$1.27 \cdot 10^{-6}$	3.01
adjoint formulation					
2	2	$6.47 \cdot 10^{-3}$		$1.99 \cdot 10^{-2}$	
4	4	$7.78 \cdot 10^{-4}$	3.06	$2.43 \cdot 10^{-3}$	3.03
8	8	$9.59 \cdot 10^{-5}$	3.02	$3.01 \cdot 10^{-4}$	3.01
16	16	$1.19 \cdot 10^{-5}$	3.01	$3.75 \cdot 10^{-5}$	3.00
32	32	$1.49 \cdot 10^{-6}$	3.00	$4.68 \cdot 10^{-6}$	3.00
64	64	$1.86 \cdot 10^{-7}$	3.00	$5.85 \cdot 10^{-7}$	3.00

Table 7: Convergence results for the primal and adjoint formulations using cubic/quadratic finite elements in time and cubic/cubic finite elements in space in the case of the smooth solution (6.1), $h_t = h_x$.

7 Conclusions

In this paper, we analyzed primal and adjoint space-time variational formulations for parabolic evolution equations using tensor product discretizations in space and time. For lowest order ansatz and test spaces, the primal formulation recovers the Crank–Nicolson method. At the same time, its space-time interpretation reveals a conditional stability property, where the stability constant depends on a CFL-type relation between the temporal and spatial mesh sizes.

This conditional stability becomes relevant in the error analysis for solutions of low regularity, in particular for discontinuous or nonsmooth initial data. The numerical experiments confirm the deteriorated behaviour of the primal method in this regime. To incorporate the initial condition differently, we derived an adjoint space-time formulation when applying integration by parts in time. For regular data, this formulation yields comparable convergence rates after a suitable postprocessing in time. For rough data, however, it shows an improved behaviour and naturally leads to a Rannacher-type smoothing of the initial data.

The Galerkin–Petrov space-time formulation therefore provides an operator-theoretic framework, based on inf-sup stability, for analyzing both classical time stepping schemes and their behaviour for nonsmooth data. For low-regularity problems, the adjoint formulation is preferable, whereas for smooth solutions the primal formulation remains competitive. Although the detailed analysis in this work was carried out for lowest order approximations, the underlying arguments extend to higher order test and ansatz spaces, as can be observed in the numerical examples.

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A Regularity estimates

In this appendix we summarize some well known results on the regularity of solutions for the initial boundary value problem (1.1), see, e.g., [15, Sect. 7.1.3]. Since the heat equation is linear, we first consider the homogeneous heat equation, and afterwards the inhomogeneous one but with zero initial conditions. We assume that $\Omega \subset \mathbb{R}^n$ is bounded with smooth boundary $\partial\Omega$, or polygonal/polyhedral but convex.

A.1 Homogeneous heat equation

We first consider the homogeneous heat equation with homogeneous Dirichlet boundary conditions, but some initial conditions,

$$\partial_t u - \Delta_x u = 0 \text{ in } Q = \Omega \times (0,T), \quad u = 0 \text{ on } \Sigma = \partial\Omega \times (0,T), \quad u(0) = u_0 \text{ in } \Omega. \tag{A.1}$$

The solution of (A.1) is given by the Fourier series

$$u(x,t) = \sum_{k=1}^{\infty} u_k \, e^{-\lambda_k t} \phi_k(x), \quad u_k = \int_\Omega u_0(x) \, \phi_k(x) \, dx, \tag{A.2}$$

where $\phi_k \in H_0^1(\Omega)$ are the normalized Dirichlet eigenfunctions of the Laplacian,

$$-\Delta \phi_k = \lambda_k \phi_k \quad \text{in } \Omega, \quad \phi_k = 0 \quad \text{on } \partial\Omega, \quad \int_\Omega \phi_k(x) \, \phi_j(x) \, dx = \delta_{kj} \, .$$

Based on (A.2) and depending on the regularity of the given initial datum u_0 we can state the following results:

Lemma A.1 *Let u as given in* (A.2) *be the solution of the initial boundary value problem* (A.1). *Depending on the regularity of the initial datum u_0 there holds:*

1. *For $u_0 \in L^2(\Omega)$ we have $u \in L^2(0,T; H_0^1(\Omega)) \cap H^1(0,T; H^{-1}(\Omega))$, satisfying*

$$\|u\|^2_{L^2(0,T;H_0^1(\Omega))} + \|u\|^2_{H^1(0,T;H^{-1}(\Omega))} \, \leq \, \|u_0\|^2_{L^2(\Omega)}, \tag{A.3}$$

   as well as $u \in H^{1,1/2}(Q) := L^2(0,T; H_0^1(\Omega)) \cap H^{1/2}(0,T; L^2(\Omega))$, satisfying

$$\|u\|^2_{L^2(0,T;H_0^1(\Omega))} + \|u\|^2_{H^{1/2}(0,T;L^2(\Omega))} \, \leq \, c \, \|u_0\|^2_{L^2(\Omega)}. \tag{A.4}$$

2. *For $u_0 \in H_0^1(\Omega)$, $u \in H^{2,1}(Q) := L^2(0,T; H^2(\Omega)) \cap H^1(0,T; L^2(\Omega))$, satisfying*

$$\|u\|^2_{L^2(0,T;H^2(\Omega))} + \|u\|^2_{H^1(0,T;L^2(\Omega))} \, \leq \, \|\nabla_x u_0\|^2_{L^2(\Omega)}. \tag{A.5}$$

3. For $u_0 \in H^1_0(\Omega) \cap H^2(\Omega)$, there holds

$$\|\nabla_x \partial_t u\|^2_{L^2(Q)} \, \leq \, \frac{1}{2} \, |u_0|^2_{H^2(\Omega)}, \tag{A.6}$$

and

$$\|u\|^2_{H^2(0,T;H^{-1}(\Omega))} \, \leq \, \frac{1}{2} \, \|u_0\|^2_{H^2(\Omega)}. \tag{A.7}$$

When using space interpolation arguments, we derive regularity results in an intermediate scale of Sobolev spaces.

Corollary A.2 *Assume $u_0 \in \widetilde{H}^s(\Omega) := [L^2(\Omega), H^1_0(\Omega)]_{|s}$ for some $s \in [0,1]$. From* (A.4) *and* (A.5) *we then conclude $u \in H^{1+s,(1+s)/2}(Q)$, and*

$$\|u\|^2_{L^2(0,T;H^{1+s}(\Omega))} + \|u\|^2_{H^{(1+s)/2}(0,T;L^2(\Omega))} \, \leq \, c \, \|u_0\|^2_{\widetilde{H}^s(\Omega)}. \tag{A.8}$$

Moreover, using (A.4) *and* (A.6) *we obtain $u \in H^{s/2}(0,T;H^1_0(\Omega))$, satisfying*

$$\|u\|_{H^{s/2}(0,T;H^1_0(\Omega))} \, \leq \, c \, \|u_0\|_{\widetilde{H}^s(\Omega)}. \tag{A.9}$$

Finally, from (A.3) and (A.7) we conclude the following estimate:

Corollary A.3 *For the solution u of* (A.1) *with $u_0 \in H^1_0(\Omega)$ there holds*

$$\|u\|^2_{H^{3/2}(0,T;H^{-1}(\Omega))} \, \leq \, c \, \|u_0\|^2_{H^1(\Omega)}. \tag{A.10}$$

A.2 Inhomogeneous heat equation

Next we consider the inhomogeneous heat equation with zero Dirichlet boundary conditions, and zero initial conditions,

$$\partial_t u - \Delta_x u = f \text{ in } Q, \quad u = 0 \text{ on } \Sigma, \quad u(0) = 0 \text{ in } \Omega. \tag{A.11}$$

The solution of (A.11) is given by the Fourier series

$$u(x,t) = \sum_{k=1}^{\infty} u_k(t) \varphi_k(x), \tag{A.12}$$

where the coefficients $u_k(t)$ are solutions of the ordinary differential equations

$$u_k'(t) + \lambda_k u_k(t) \, = \, f_k(t) \, := \, \langle f(t), \varphi_k \rangle_\Omega \quad \text{for } t \in (0,T), \quad u_k(0) = 0.$$

Lemma A.4 *Let u as given in* (A.12) *be the solution of the initial boundary value problem* (A.11). *Depending on the regularity of f there holds:*

1. *For $f \in L^2(0,T;H^{-1}(\Omega))$, we have $u \in L^2(0,T;H^1_0(\Omega)) \cap H^1_{0,}(0,T;H^{-1}(\Omega))$, with*

$$\|u\|^2_{L^2(0,T;H^1_0(\Omega))} + \|u\|^2_{H^1(0,T;H^{-1}(\Omega))} \le 2\,\|f\|^2_{L^2(0,T;H^{-1}(\Omega))}, \tag{A.13}$$

as well as $u \in H^{1,1/2}_{0;0,}(Q) := L^2(0,T;H^1_0(\Omega)) \cap H^{1/2}_{0,}(0,T;L^2(\Omega))$, satisfying

$$\|u\|^2_{L^2(0,T;H^1_0(\Omega))} + \|u\|^2_{H^{1/2}_{0,}(0,T;L^2(\Omega))} \le 2\,\|f\|^2_{L^2(0,T;H^{-1}(\Omega))}. \tag{A.14}$$

2. *For $f \in L^2(Q)$, $u \in L^2(0,T;H^1_0(\Omega) \cap H^2(\Omega)) \cap H^1_{0,}(0,T;L^2(\Omega))$, satisfying*

$$\|u\|^2_{L^2(0,T;H^1_0(\Omega)\cap H^2(\Omega))} + \|u\|^2_{H^1_{0,}(0,T;L^2(\Omega))} \le 2\,\|f\|^2_{L^2(Q)}. \tag{A.15}$$

3. *For $f \in L^2(0,T;H^1_0(\Omega))$, there holds*

$$\|\nabla_x \partial_t u\|^2_{L^2(Q)} \le \|f\|^2_{L^2(0,T;H^1_0(\Omega))}. \tag{A.16}$$

4. *If $f \in H^1_{0,}(0,T;H^{-1}(\Omega))$ is satisfied, then*

$$\|\partial_{tt} u\|_{L^2(0,T;H^{-1}(\Omega))} \le \sqrt{2}\,\|f\|_{H^1(0,T;H^{-1}(\Omega))}. \tag{A.17}$$

Again we can use space interpolation arguments to formulate regularity results in an intermediate scale of Sobolev spaces. From (A.14) and (A.15) we have:

Corollary A.5 *Assume $f \in L^2(0,T;H^{-1+s}(\Omega)) := [L^2(0,T;H^{1-s}_0(\Omega))]^*$ for some $s \in [0,1]$. Then, we conclude $u \in H^{1+s,(1+s)/2}(Q)$, and*

$$\|u\|^2_{L^2(0,T;H^{1+s}(\Omega))} + \|u\|^2_{H^{(1+s)/2}(0,T;L^2(\Omega))} \le c\,\|f\|^2_{L^2(0,T;H^{-1+s}(\Omega))}. \tag{A.18}$$

Finally, from (A.13) and (A.17) we conclude the following estimate:

Corollary A.6 *For the solution u of* (A.11) *with $f \in H^{1/2}_{0,}(0,T;H^{-1}(\Omega))$ there holds*

$$\|u\|^2_{H^{3/2}(0,T;H^{-1}(\Omega))} \le c\,\|f\|^2_{H^{1/2}(0,T;H^{-1}(\Omega))}. \tag{A.19}$$

B Equivalence of inf-sup stability constants

Because for any bounded, linear isomorphism $B : X \to Y^*$ it holds that $(B^{-1})^* = (B^*)^{-1}$, and $\|B\|_{X\to Y^*} = \|B^*\|_{Y\to X^*}$, the continuous inf-sup constants for B and B^* are the same, i.e.,

$$\inf_{0\neq u\in X}\sup_{0\neq v\in Y}\frac{\langle Bu,v\rangle_{Y^*\times Y}}{\|u\|_X\|v\|_Y} = \inf_{0\neq v\in Y}\sup_{0\neq u\in X}\frac{\langle B^*v,u\rangle_{X^*\times X}}{\|u\|_X\|v\|_Y}.$$

The same conclusion holds true for the discrete inf-sup constant, e.g., [8, Proposition 3.4.3]. For completeness, and because our discrete trial and test spaces differ slightly, we include a proof of this result in the next lemma.

Lemma B.1 *It holds that*

$$\inf_{0\neq u_h\in X_{0,h}} \sup_{0\neq v_h\in Y_h} \frac{b(u_h,v_h)}{\|u_h\|_X\|v_h\|_Y} = \inf_{0\neq v_h\in Y_h} \sup_{0\neq u_h\in X_{T,h}} \frac{b_T(v_h,u_h)}{\|v_h\|_Y\|u_h\|_X},$$

where $b(\cdot,\cdot) : X_{0,h}\times Y_h \to \mathbb{R}$ *and* $b_T(\cdot,\cdot) : Y_h\times X_{T,h}\to\mathbb{R}$ *are defined in* (2.2) *and* (5.1), *respectively.*

Proof. We first note that the time reversal map $\iota_T v(t) := v(T-t)$, when solely acting on time, is an isometric isomorphism as a map $\iota_T : Y_h \to Y_h$, and as a map $\iota_T : X_{0,h}\to X_{T,h}$. Moreover, $\partial_t\iota_T = -\iota_T\partial_t$, $\iota_T^2 = \mathrm{id}$, and the L^2 adjoint satisfies $\iota_T^* = \iota_T$. Hence, for all $u\in X_0$ and $v\in Y$ we have that

$$\begin{aligned}
b(u,v) &= \int_0^T\int_\Omega \Big[\partial_t u(x,t)\, v(x,t) + \nabla_x u(x,t)\cdot\nabla_x v(x,t)\Big]\,dt\,dx\\
&= \int_0^T\int_\Omega \Big[\partial_t u(x,t)\, \iota_T^2 v(x,t) + \nabla_x u(x,t)\cdot\nabla_x \iota_T^2 v(x,t)\Big]dt\,dx\\
&= \int_0^T\int_\Omega \Big[\iota_T^*\partial_t u(x,t)\, \iota_T v(x,t) + \nabla_x \iota_T^* u(x,t)\cdot\nabla_x \iota_T v(x,t)\Big]dt\,dx\\
&= \int_0^T\int_\Omega \Big[\iota_T\partial_t u(x,t)\, \iota_T v(x,t) + \nabla_x \iota_T u(x,t)\cdot\nabla_x \iota_T v(x,t)\Big]dt\,dx\\
&= \int_0^T\int_\Omega \Big[-\partial_t \iota_T u(x,t)\, \iota_T v(x,t) + \nabla_x \iota_T u(x,t)\cdot\nabla_x \iota_T v(x,t)\Big]dt\,dx\\
&= b_T(\iota_T v, \iota_T u).
\end{aligned}$$

Thus, for the operators $B_{0,h} : X_{0,h}\to Y_h^*$, and $B_{T,h} : Y_h \to X_{T,h}^*$, defined as

$$\langle B_{0,h}u_h, v_h\rangle_{Y^*\times Y} = b(u_h,v_h), \quad \langle B_{T,h}v_h, u_h\rangle_{X^*\times X} = b_T(v_h,u_h),$$

there holds the relation

$$\begin{aligned}
\langle B_{0,h}u_h, v_h\rangle_{Y^*\times Y} &= b(u_h,v_h) = b_T(\iota_T v_h, \iota_T u_h)\\
&= \langle B_{T,h}\iota_T v_h, \iota_T u_h\rangle_{X^*\times X} = \langle \iota_T^* B_{T,h}^*\iota_T u_h, v_h\rangle_{Y^*\times Y}
\end{aligned}$$

for all $u_h\in X_{0,h}$, and $v_h\in Y_h$, i.e., $B_{0,h} = \iota_T^* B_{T,h}^*\iota_T$. Now, we compute the discrete inf-sup constant for the primal problem as

$$\begin{aligned}
\inf_{0\neq u_h\in X_{0,h}} \sup_{0\neq v_h\in Y_h} \frac{b(u_h,v_h)}{\|u_h\|_X\|v_h\|_Y} &= \inf_{0\neq u_h\in X_{0,h}} \sup_{0\neq v_h\in Y_h} \frac{\langle B_{0,h}u_h, v_h\rangle_{Y^*\times Y}}{\|u_h\|_X\|v_h\|_Y}\\
&= \inf_{0\neq u_h\in X_{0,h}} \frac{\|B_{0,h}u_h\|_{Y^*}}{\|u_h\|_X}.
\end{aligned}$$

Moreover,

$$\begin{aligned}
\inf_{0\neq u_h\in X_{0,h}} \frac{\|B_{0,h}u_h\|_{Y^*}}{\|u_h\|_X} &= \inf_{0\neq v_h\in Y_h^*} \frac{\|v_h\|_{Y^*}}{\|B_{0,h}^{-1}v_h\|_X} \\
&= \left(\sup_{0\neq v_h\in Y_h^*} \frac{\|B_{0,h}^{-1}v_h\|_X}{\|v_h\|_{Y^*}}\right)^{-1} = \|B_{0,h}^{-1}\|_{Y_h^*\to X_{0,h}}^{-1}.
\end{aligned}$$

Using that $\|B_{0,h}^{-1}\|_{Y_h^*\to X_{0,h}} = \|B_{0,h}^{-1,*}\|_{X_{0,h}^*\to Y_h}$, and that $B_{0,h}^{-1,*} = B_{0,h}^{*,-1} = (\iota_T^* B_{T,h}\iota_T)^{-1}$, we then compute

$$\begin{aligned}
\|B_{0,h}^{-1}\|_{Y_h^*\to X_{0,h}}^{-1} &= \|(\iota_T^* B_{T,h}\iota_T)^{-1}\|_{X_{0,h}^*\to Y_h}^{-1} \\
&= \inf_{0\neq v_h\in Y_h} \sup_{0\neq u_h\in X_{0,h}} \frac{\langle B_{T,h}\iota_T v_h, \iota_T u_h\rangle_{X^*\times X}}{\|u_h\|_X\|v_h\|_Y} \\
&= \inf_{0\neq v_h\in Y_h} \sup_{0\neq u_h\in X_{0,h}} \frac{b_T(\iota_T v_h, \iota_T u_h)}{\|u_h\|_X\|v_h\|_Y} \\
&= \inf_{0\neq v_h\in Y_h} \sup_{0\neq u_h\in X_{T,h}} \frac{b_T(v_h, u_h)}{\|u_h\|_X\|v_h\|_Y}.
\end{aligned}$$

This concludes the proof. ■