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Estimates of the Rate of Convergence for Distributed Parameter Identification in Linear Parabolic Problems*

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Abstract

The identification problem of diffusion coefficient in the homogenous, parabolic equation is considered. For this purpose, methods are introduced which use the well-known output least squares idea with modifications. For the proposed methods, both semidiscrete and fully discrete estimates of the rate of convergence are proved, when the finite element and Crank-Nicolson methods are applied. Some numerical results are included.

Key words: parameter identification, parabolic problem, finite element method, estimates of the rate of convergence

AMS Subject Classifications: 65M60, 49N50, 35B37

1 Introduction

In this article, we consider the homogenous, parabolic equation

$$
\begin{aligned}
\frac{\partial u(t,x)}{\partial t} - \nabla \cdot (b(t,x)\, \nabla u(t,x)) &= f(t,x) \quad \text{in } [0,T] \times \Omega\,, \\
u\big|_{\Gamma_0} = \frac{\partial u}{\partial n}\bigg|_{\Gamma_1} &= 0 \quad \text{in } [0,T]\,, \\
u(0,x) &= u_0(x) \quad \text{in } \Omega\,,
\end{aligned}
\tag{1.1}
$$

where Ω is a bounded domain in $\mathbb{R}^d$, $d \leq 3$, with smooth boundary $\partial\Omega = \overline{\Gamma_0} \cup \overline{\Gamma_1}$. Γ_0 and Γ_1 are open disjoint subsets of $\partial\Omega$, and $[0,T]$ is a fixed time interval with $T < \infty$. A direct problem in (1.1) consists of finding the unknown solution u when we know functions b, f, and u_0, but here we are

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interested in the corresponding inverse problem: with some information about the solution u recover the parameter b.

We assume that we have two distributed observations: z of the solution u and ϕ of $\frac{\partial u}{\partial t}$. In practice, we can usually measure observations in some points of the domain Ω at different time levels, i.e., we have a discrete observation of the form $u(t_j, x_i), j = 0, ..., n,\ i = 0, ..., m$. After interpolating this point data we get a distributed observation for both u and $\frac{\partial u}{\partial t}$ with some interpolation and measurement errors. Notice that if it is (physically) possible to set up the measurement points as we like, we can take these points to be the same as the discretization points used in the computations. In this way, the observation functions are already in a discrete form (interpolants from point-wise values using a discrete basis). Moreover, the same is true, if we first interpolate values from the measurements points to the discretization points. The third possibility, if we have enough observation points, is to make the triangulation of the domain so that the observations points are exactly vertices of the elements. In this case, however, the triangulation should be regular and quasi-uniform, which cannot be ensured with arbitrary measurement points. Anyway, because of this practical consideration, it is reasonable to assume that our observations are initially discrete functions which are defined in a suitable basis.

With the given observations we use first the output least squares method to transform the identification problem of b to a minimization problem. The main idea of this work is to include extra terms to the least squares cost functional, which take into account the underlying equation (1.1). For elliptic identification problems, similar methods are presented in [16] and [12]. Moreover, the well-known augmented Lagrangian formulation of the identification problem ([13] and articles therein) can lead to a very similar approximation. However, at least we do not know any other work, where estimates of the rate of convergence for a general finite element approximation of linear parabolic identification problems are given. In [11] we proved a semidiscrete error estimate for a parabolic identification problem, but essentially with a different technique, because in [11] the governing equation with Neumann boundary conditions was quasilinear and the identified parameter nonlinear. We can notice that also in [11] the availability of observations for both u and $\frac{\partial u}{\partial t}$ was assumed.

In fact, with the proposed method one identifies b by minimizing

$$J(u,b) = \|u - z\|_V^2 + \delta(\|\frac{\partial u}{\partial t} - \phi\|_H^2 + \|\frac{\partial u}{\partial t} - \nabla \cdot (b\nabla u) - f\|_H^2) \tag{1.2}$$

for suitable norms V and H. For obvious reasons, namely the different amount of differentiation which will be included in the cost functional, δ must depend on the discretization parameter h (in our case $\delta = h^4$ or h^2). This means that when h (δ) tends to zero, (u, b) converge to the output least squares solution of the identification problem. In our case, for fixed $h > 0$, the extra terms included improve the convexity properties of the cost functional near the minimum, and the existence of a minimizer over a non-empty, closed and convex set of admissible pairs (u, b) follows. However, because we solve the original equation (1.1) in a discrete form during the minimization process, we have actually $u = u(b)$ and $J(u, b) = J(b)$. Therefore, the price we must pay for this improvement is the more complicated right-hand side of the adjoint equation, which is solved to find the gradient of the cost functional with respect to b. If we would like to avoid this, we can regard u and b as separate variables (like in the augmented Lagrangian method) without solving any state equation. The weakness of this approach compared to our method is the fact that it needs the minimization over a larger space $V \times M$ ($u \in V,\ b \in M$). Nevertheless, from the following error analysis it is easy to see that the same error estimates between the true and the computed parameter remain valid, if u and b are treated separately in the cost functional. Because of the computational simplicity, the numerical examples will be computed in this way.

The error analysis of the parabolic inverse problem will be based on the techniques used for the corresponding direct problems. Useful references for our work have been, for example, the books [2], [3], and the papers [7], [8], and [9].

Standard notations for Sobolev spaces and associated norms will be used. We regard C as a generic constant which may vary in different contexts, but is always independent of the discretization parameter h. From now on we denote by D_t the derivative with respect to time variable t.

This paper is organized as follows. In section 2, we formulate the identification problem as an optimal control problem by introducing cost functionals which are minimized in the computational procedure. This is followed by estimates of the rate of convergence when equation (1.1) is semidiscretized with the finite element method. In section 3, we analyze a fully discrete case when the discretization in time is made with the Crank-Nicolson scheme. In section 4, we give some numerical results which are computed with the proposed methods. For theorems in sections 2 and 3 we need a few preliminary lemmas. Proofs of these lemmas are quite lengthy, so we include them in the Appendix at the end of the paper.

2 Error Estimates for the Semidiscrete Problem

In order to define the finite element spaces, let $\mathcal{T}_h, 0 < h < 1$, be a family of triangulations of $\bar{\Omega}$. If the boundary of Ω is curved, we use either isoparametric elements ([1]) or triangles with one edge replaced by the curved segment of the boundary ([6]). We assume that the family $\mathcal{T}_h$ is regular and quasi-uniform. For fixed integers $r \geq 1, l \geq 0$, we define a finite element space as

$$S^r_{h,l} = \left\{ v \mid v \in C^{l-1}(\bar{\Omega}),\ \ v|_T \in P_r \ \forall\ T \in \mathcal{T}_h \right\}, \tag{2.1}$$

where P_r is the space of polynomials of degree less than or equal to r. By $S^{r,0}_{h,l}$ we denote the subspace of $S^r_{h,l}$ of functions which vanish on $,_0 \subset \partial\Omega$.

The parabolic equation (1.1) in a weak Galerkin form states as follows: find $u = u(t) : [0,T] \to \widetilde{H}^1(\Omega)$ such that

$$\begin{aligned} (D_t u, v) + (b\,\nabla u, \nabla v) &= (f, v) \quad \forall v \in \widetilde{H}^1(\Omega)\,, \\ u(0,x) &= u_0(x) \quad \text{in } \Omega\,, \end{aligned} \tag{2.2}$$

where

$$\widetilde{H}^1(\Omega) = \left\{ v \in H^1(\Omega) \mid \ v|_{,_0} = 0 \right\}. \tag{2.3}$$

The semidiscrete finite element approximation of (2.2) reads: find $u_h = u_h(t) : [0,T] \to U_h$ such that

$$\begin{aligned} (D_t u_h, v_h) + (b\,\nabla u_h, \nabla v_h) &= (f, v_h) \quad \forall v_h \in U_h\,, \\ u(0,x) &= u_{0,h} \quad \text{in } \Omega\,, \end{aligned} \tag{2.4}$$

where $u_{0,h}$ is the interpolant of u_0 in $U_h \subset \widetilde{H}^1$.

If v is a strongly measurable map of $(0,T)$ into the Banach space X with a norm $\|\cdot\|_X$, we set

$$\|v\|^2_{L^2((0,T);X)} = \|v\|^2_{L^2(X)} = \int_0^T \|v(s)\|^2_X \, ds\,. \tag{2.5}$$

Moreover, if v is continuous from $[0,T]$ into X, we take

$$\|v\|_{C^0([0,T];X)} = \|v\|_{C^0(X)} = \sup_{t \in [0,T]} \|v(t)\|_X\,. \tag{2.6}$$

By $\widetilde{H}^{-1}$ we denote the dual space of $\widetilde{H}^1$ equipped with the natural norm

$$\|v\|_{-1} = \sup_{\substack{\psi \in \widetilde{H}^1 \\ \psi \neq 0}} \frac{|(v,\psi)|}{\|\psi\|_1}\,. \tag{2.7}$$

Then, for $v \in \widetilde{H}^{-1}$ and $\psi \in \widetilde{H}^1$, we have an inequality

$$|(v,\psi)| \le \|v\|_{-1} \|\psi\|_1\,. \tag{2.8}$$

We assume the following smoothness of the functions in (1.1)

$$\begin{aligned} &u \in C^0(\widetilde{H}^1 \cap W^{2,\infty} \cap H^{r+1}) \cap L^2(H^{r+2})\,, D_t u \in C^0(H^{r-1}), \\ &b \in C^0(H^r \cap W^{1,\infty}) \cap L^2(H^{r+1}),\ \text{and}\ f \in C^0(H^{r-1}) \end{aligned} \tag{2.9}$$

for $r \geq 2$. For the computational procedure, we introduce four discretization spaces: U_h for the solution u, B_h for the parameter b, Z_h for the observations z_h and ϕ_h, and finally F_h which is used to discretize the right-hand side f. We choose

$$U_h = S_{h,2}^{r+1,0}\,,\ B_h = S_{h,1}^{r}\,,\ Z_h = S_{h,1}^{r+1,0}\,,\ F_h = S_{h,0}^{r-2}\,. \tag{2.10}$$

Let $z_h(t,x)$ be the distributed L^2-observation of the state u and $\phi_h(t,x)$ of $D_t u$ at each time level t. As explained in the introduction, we assume that these observations are given already in the discrete space Z_h. Notice that because z_h observes u (without an observation error z_h is nothing more than the interpolant of u in Z_h), the degree of local interpolation polynomials in Z_h depends on the regularity of u. Moreover, because we do not want to define an extra discrete space for ϕ_h (just to keep the presentation clearer), we use Z_h for this observation as well. We assume that the observation error takes the form

$$\begin{aligned} \|u - z_h\|_0 &\leq \varepsilon_1\,, \\ \|D_t u - \phi_h\|_0 &\leq \varepsilon_2\,, \end{aligned} \tag{2.11}$$

for all $t \in [0,T]$.

The cost functional to be minimized is defined as

$$\begin{aligned} J(b_h) &= \sup_{t\in[0,T]} \Big\{ \|u_h(b_h) - z_h\|_0^2 + h^4 \Big(\|D_t u_h(b_h) - \phi_h\|_0^2 \\ &\qquad + \|D_t u_h(b_h) - \nabla\cdot(b_h\,\nabla u_h(b_h)) - f_h\|_0^2 \Big) \Big\}\,. \end{aligned} \tag{2.12}$$

Here, $u_h(b_h) = u_h(b_h)(t)$ is the solution of (2.4) with the parameter $b_h = b_h(t,x)$, $z_h = z_h(t,x)$ and $\phi_h = \phi_h(t,x)$ are the given observations in Z_h, and $f_h = f_h(t,x)$ is the interpolant of $f(t,x)$ in F_h. We see that all functions in (2.12) are piecewise polynomials. This is to ensure that we can compute the cost functional by applying a suitable quadrature formula. As explained in the introduction, $J(b_h)$ can be seen as a weighted combination of output least squares and equation error cost functionals.

The actual identification problem is of the form:

$$\text{find } b_h \in M_h :\ J(b_h) \leq J(\tilde b_h) \quad \forall\ \tilde b_h \in M_h\,, \tag{2.13}$$

where

$$\begin{aligned} M = \ & \Big\{ \tilde b \in C^0([0,T]; H^1 \cap L^\infty) \mid 0 < \lambda_1 \leq \tilde b(t) \leq \lambda_2 < \infty \text{ a.e. in } \Omega\,, \\ & \|\nabla \tilde b(t)\|_0 \leq \mu < \infty\ \forall t \in [0,T] \Big\} \end{aligned} \tag{2.14}$$

is the set for admissible parameters with given positive constants $\lambda_1, \lambda_2, \mu \in \mathbb{R}$, and $M_h = M \cap B_h$ for all $t \in [0,T]$. Using the well-known theory of lower semicontinuous functionals the existence of a solution b_h for (2.13) follows.

We require that the true parameter $b = b(t,x)$ satisfies

$$\begin{aligned} \lambda_1 < b(t) &\quad < \lambda_2 \text{ a.e in } \Omega\,, \\ \|\nabla b(t)\|_0 &\quad < \mu\,, \end{aligned} \tag{2.15}$$

$\forall t \in [0,T]$. Notice that the first condition assumed in (2.15) is exactly of the same form as in the Falk's paper ([14]), which contains error estimates for an elliptic identification problem. The second assumption in (2.15) follows naturally from the structure of set M (which in our case is different from [14]), as we can see from the proof of Lemma 2.2. The reason for this assumption is the technical fact that we must find an element from the discrete space B_h which is close to b and belongs to the set M_h of discrete admissible parameters. For this purpose, we need b to be isolated from the constraints in M.

Let us first state some lemmas which are proved in the Appendix.

Lemma 2.1 *Between the solution $u = u(b)(t)$ of (1.1) and the solution $u_h = u_h(b)(t)$ of (2.4) we have estimates*

$$\begin{aligned} \|u - u_h\|_{C^0(H^k)} &\leq C\, h^{r+1-k} \quad \textit{for } k = 0,1\,, \\ \|u - u_h\|_{L^2(H^1)} &\leq C\, h^{r+1}\,, \\ \|D_t(u - u_h)\|_{C^0(\widetilde{H}^{-1})} &\leq C\, h^r\,, \\ \|D_t(u - u_h)\|_{C^0(L^2)} &\leq C\, h^{r-1}\,. \end{aligned}$$

Lemma 2.2 *For all $t \in [0,T]$, let θ_h be the L^2-projection of b into B_h, and $u_h(\theta_h)$ the corresponding state which is calculated from (2.4). Then, for h small enough, $\theta_h \in M_h$, and we have*

$$\begin{aligned} \|u_h(\theta_h) - u\|_{C^0(H^k)} &\leq C\, h^{r+1-k} \quad \textit{for } k = 0,1\,, \\ \|D_t(u_h(\theta_h) - u)\|_{C^0(\widetilde{H}^{-1})} &\leq C\, h^r\,, \\ \|D_t(u_h(\theta_h) - u)\|_{C^0(L^2)} &\leq C\, h^{r-1}\,. \end{aligned}$$

Lemma 2.3 *Between the solution $u = u(b)(t)$ of (1.1) and the solution $w_h = u_h(b_h)(t)$ of (2.4) which corresponds to a minimizer b_h of $J(b_h)$, we have, for h small enough, estimates*

$$\begin{aligned} &\|w_h - u\|_{C^0(H^k)} \leq C\, h^{-k}\,(h^{r+1} + \varepsilon_1 + h^2\,\varepsilon_2) \quad \textit{for } 0 \leq k \leq 2\,, \\ &\|D_t(w_h - u)\|_{C^0(L^2)} \leq C\,(h^{r-1} + h^{-2}\,\varepsilon_1 + \varepsilon_2)\,, \\ &\|D_t w_h - \nabla \cdot (b_h\, \nabla w_h) - f\|_{C^0(L^2)} \leq C\,(h^{r-1} + h^{-2}\,\varepsilon_1 + \varepsilon_2)\,. \end{aligned}$$

Theorem 2.1 *There exists a constant $C > 0$ independent of h, such that, between the original parameter b and the calculated parameter b_h, an estimate*

$$\int_\Omega |b(t) - b_h(t)||\nabla u(t)|^2 \, dx \leq C \left(h^{r-1} + h^{-2}\varepsilon_1 + \varepsilon_2 \right)$$

is valid, for h sufficiently small and $\forall t \in [0, T]$.

Proof: By (1.1) and the regularity of our functions, the following equation between $b(t), u(t)$ and $b_h(t), w_h(t)$ is valid in $L^2(\Omega)$ for all $t \in [0, T]$:

$$\begin{aligned} &-\nabla \cdot ((b(t) - b_h(t)) \, \nabla u(t)) \\ &= -D_t u(t) + f(t) + \nabla \cdot (b_h(t) \, \nabla u(t)) \\ &= D_t(w_h(t) - u(t)) - D_t w_h(t) + \nabla \cdot (b_h(t) \, \nabla w_h(t)) + f(t) \\ &-\nabla \cdot (b_h(t) \, \nabla (w_h(t) - u(t))) \, . \end{aligned} \tag{2.16}$$

We proceed now with the technique introduced in [13]. For fixed $t \in [0, T]$, let us define two disjoint subsets of Ω, such that $R_1 = \{x \in \Omega : b(t, x) - b_h(t, x) \geq 0\}$ and $R_2 = \Omega - R_1$. Let the function $\psi(t) \in L^\infty(\Omega)$ be as $\psi(t) = 1$ in R_1 and $\psi(t) = -1$ in R_2. Now, by taking the L^2-inner product of (2.16) with $\psi(t)u(t) \in L^\infty(\Omega)$ we get

$$\begin{aligned} &-(\nabla \cdot (|b(t) - b_h(t)| \, \nabla u(t)), u(t)) \\ &= (D_t(w_h(t) - u(t)) - (D_t w_h(t) - \nabla \cdot (b_h(t) \, \nabla w_h(t)) - f(t)) \\ &\quad -\nabla \cdot (b_h(t) \, \nabla (w_h(t) - u(t))), \psi(t) u(t)) \, . \end{aligned} \tag{2.17}$$

Since $b(t)$ and $b_h(t)$ are both in $C^0(H^1)$, $|b(t) - b_h(t)| \, \nabla u(t) \in C^0(H^1)$ as a consequence of $u \in C^0(W^{2,\infty})$. Hence, an application of Green's formula together with the boundedness of $b_h(t)$ in $C^0(H^1 \cap L^\infty)$ and $\psi(t)u(t)$ in $C^0(L^\infty)$ shows

$$\begin{aligned} &\int_\Omega |b(t) - b_h(t)| \, |\nabla u(t)|^2 \, dx \\ &\leq C \, (\|D_t(w_h(t) - u(t))\|_0 + \|D_t w_h(t) - \nabla \cdot (b_h(t) \, \nabla w_h(t)) - f(t)\|_0 \\ &\quad + \|w_h(t) - u(t)\|_2) \end{aligned} \tag{2.18}$$

$\forall t \in [0, T]$. The result follows now from Lemma 2.3.

Next we will use the estimate of Lemma 2.2 established in $\widetilde{H}^{-1}$. In the case $d = 1$ the domain Ω reduces to an interval $I = (a, b)$. From now on we assume that at least on one end of the interval we have a Neumann condition $u'(a) = 0$ or $u'(b) = 0$. Moreover, because $U_h \subset C^1(\bar{I})$, we can take the discrete solution $u_h(t)$ of (2.4) to satisfy also the homogenous Neumann boundary conditions exactly while the test function space $\widetilde{H}^1$

is kept as before. Notice that in this way the so-called Petrov-Galerkin procedure (discrete spaces for solutions and test functions are different) for solving (1.1) is defined ([15], Chapter 5), for which the estimates in Lemmas 2.1 and 2.2 remain valid.

We define a new cost functional as

$$\begin{aligned}\tilde{J}(b_h) \quad &= \sup_{t\in[0,T]} \Big\{ \|u_h(b_h) - z_h\|_0^2 + h^2 \Big(\|D_t u_h(b_h) - \phi_h\|_{-1}^2 \\ &\qquad + \|D_t u_h(b_h) - (b_h\, u_h'(b_h))' - f\|_{-1}^2 \Big) \Big\} \,, \end{aligned} \tag{2.19}$$

where $'$ denotes the differentiation with respect to x-variable and the last two norms are realized in the dual space $\widetilde{H}^{-1}$. The new cost functional (2.19) is introduced, because we can improve the convergence estimate of Theorem 2.1 in this special case. Moreover, to consider the last two terms in (2.19) in $\widetilde{H}^{-1}$-norm means that we must solve two additional Laplace or Helmholz equations with suitable boundary conditions in order to compute these terms (see Lemma 3.4 in section 3).

Theorem 2.2 *Assume that* (2.9), (2.11), (2.15) *hold and* $d = 1$. *Then, there exists a constant* $C > 0$ *independent of* h, *such that an error estimate*

$$\|(b - b_h)\, u'\|_{C^0(L^2)} \leq C\,(h^r + h^{-1}\,\varepsilon_1 + \varepsilon_2)$$

between the original parameter $b = b(t,x)$ *and a minimizer* $b_h = b_h(t,x)$ *of* (2.19) *is valid, for* h *sufficiently small.*

Proof: For simplicity, we write the functions here without the variable (t,x). First, however, let us fix $t \in [0,T]$. A weak form of equation (2.16) reads as

$$\begin{aligned}((b-b_h)\,u', v') \quad &= (D_t(w_h - u), v) + (-D_t w_h + (b_h\, w_h')' + f, v) \\ &\quad + (b_h\,(w_h - u)', v') \quad \forall v \in \widetilde{H}^1 \,, \end{aligned} \tag{2.20}$$

because also w_h satisfies the boundary conditions exactly. Since $\widetilde{H}^1$ is now either the whole space H^1 or its subspace of the form

$$\widetilde{H}^1 = \big\{ v \in H^1 \,|\, v(e) = 0 \big\} \tag{2.21}$$

for e equal to a or b, we can define the test function $v \in \widetilde{H}^1$ as a solution of the boundary value problem

$$\begin{cases} v'(x) &= [(b-b_h)\,u'](x), \quad x \in I \,, \\ v(e) &= 0 \,. \end{cases} \tag{2.22}$$

So, using this v in (2.20) and applying (2.8)

$$\begin{aligned}\|(b-b_h)\,u'\|_0^2 &\le C\,(\|D_t(w_h-u)\|_{-1}+\|D_tw_h-(b_h\,w_h')'-f\|_{-1}\\ &\quad+\|b_h\,(w_h-u)'\|_0)\,\|v'\|_0\\ &\le C\,(\|D_t(w_h-u)\|_{-1}+\|D_tw_h-(b_h\,w_h')'-f\|_{-1}\\ &\quad+\|(w_h-u)'\|_0)\,\|(b-b_h)\,u'\|_0\,. \end{aligned} \tag{2.23}$$

A direct calculation shows that in the dual space $\widetilde{H}^{-1}$ we have

$$\|(a\,g')'\|_{-1}\le\|a\,g'\|_0\,, \tag{2.24}$$

when g satisfies the boundary conditions in (1.1). Finally, using (2.19) and (2.24) we have, like in the proof of Lemma 2.3

$$\begin{aligned}&\|w_h-z_h\|_0^2+h^2\,(\|D_tw_h-\phi_h\|_{-1}^2+\|D_tw_h-(b_h\,w_h')'-f\|_{-1}^2)\\ &\le\|u_h(\theta_h)-z_h\|_0^2+h^2\,(\|D_tu_h(\theta_h)-\phi_h\|_{-1}^2\\ &\quad+\|D_tu_h(\theta_h)-(\theta_h\,u_h'(\theta_h))'-f\|_{-1}^2)\\ &\le 2(\|u_h(\theta_h)-u\|_0^2+\|u-z_h\|_0^2)\\ &+2h^2\,(\|D_t(u_h(\theta_h)-u)\|_{-1}^2+\|D_tu-\phi_h\|_{-1}^2)\\ &+h^2\|D_tu_h(\theta_h)-(\theta_h\,u_h'(\theta_h))'-D_tu+(b\,u')'\|_{-1}^2\\ &\le C\,(h^{2(r+1)}+\varepsilon_1^2+h^2\,\varepsilon_2^2)+h^2\,(\|D_t(u_h(\theta_h)-u)\|_{-1}^2\\ &\quad+\|(\theta_h\,(u-u_h(\theta_h))')'\|_{-1}^2+\|((b-\theta_h)\,u')'\|_{-1}^2)\\ &\le C\,(h^{2(r+1)}+\varepsilon_1^2+h^2\,\varepsilon_2^2)+h^2\,(\|u-u_h(\theta_h)\|_1^2+\|b-\theta_h\|_0^2)\\ &\le C\,(h^{2(r+1)}+\varepsilon_1^2+h^2\varepsilon_2^2)\,. \end{aligned} \tag{2.25}$$

Since t was fixed, (2.20) - (2.25) hold for all $t\in[0,T]$. Therefore, exactly as in (5.49), we get

$$\begin{aligned}\|w_h-u\|_{C^0(L^2)} &\le C\,(h^{r+1}+\varepsilon_1+h\,\varepsilon_2)\,,\\ \|D_t(w_h-u)\|_{C^0(\widetilde{H}^{-1})} &\le C\,(h^r+h^{-1}\,\varepsilon_1+\varepsilon_2)\,,\\ \|D_tw_h-(b_h\,w_h')'-f\|_{C^0(\widetilde{H}^{-1})} &\le C\,(h^r+h^{-1}\,\varepsilon_1+\varepsilon_2)\,. \end{aligned} \tag{2.26}$$

Hence, the result follows from (2.23) and (2.26) with the inverse inequality.

Remark 2.1 It is clear that the most stringent requirement in our theory is to have a C^1 finite element space for discretizing u. Of course, this is not a problem in $1d$ or in the case when a tensor product basis can be used for $d=2,\ 3$. However, there might be a possibility to overcome this problem by introducing a new, vector-valued variable σ for the flux $a\nabla u$, i.e., by using a mixed formulation of the original problem (1.1) (see, e.g.,

[15], Chapter 7). For elliptic identification problems, an approach using the mixed formulation is introduced and analyzed in [16].

Moreover, from the proof of Theorem (2.2) we notice that if w_h does not satisfy the Neumann boundary conditions exactly, a boundary term to evaluate will appear in (2.20). Using the trace theorem for Sobolev spaces, this suggests that in this case the error estimate of Theorem (2.2) should be multiplied by $h^{-\frac{1}{2}}$. Of course, this is also valid for our discrete estimate in the next section as well. However, our numerical computations in section 4 do not indicate such phenomenon. Therefore, to prove an improved estimate using only C^0 discretization remains as a future challenge.

Remark 2.2 Why not pure output least squares method? As we can see from our theorems, their proofs are based on the fact that we can write an error equation between the true and the computed parameter in a strong form ((2.16), (2.20)). The additional error equation term in the cost functionals enables to use this kind of technique (in fact, this is exactly the reason why we included these terms to the cost functionals at first place). With output least squares method we can not do this, because only the equation which is satisfied for b_h and $u_h(b_h)$ is the weak Galerkin form (2.4) with only discrete functions.

To get a strong equation which can be used in the error analysis, the first idea, of course, is to define a strong solution $u(b_h)$ of the original equation (1.1) with the discrete parameter b_h. But then the difficulty is the following: for an error estimate between b and b_h we must have estimates between $u(b_h)$ and $u_h(b_h)$. But, as we know very well, these estimates depend on the regularity of $u(b_h)$ which depends on the regularity of the discrete parameter b_h. So the higher order estimates we want to have the higher regularity we must assume for b_h. Computationally this is very restrictive, because we need discrete spaces which are subspaces of high order Sobolev Spaces ($H^2(\Omega)$ or more). Moreover, the boundedness of the discrete parameter (and its time derivatives) in these spaces is a nonlinear constraint which must be taken into account in the optimization. From our results we see that higher order estimates are obtained without any change in the set M of admissible parameters and the regularity of the discrete parameter b_h.

3 Estimates for the Fully Discrete Scheme

First we fix some notations. Let $1 \leq m \in \mathbb{N}$ be a positive integer and set $\Delta t = \frac{T}{m}$. We divide the time-axis $[0,T]$ into subintervals $[t_j, t_{j+1}], j = 0, ..., m-1$, where $t_j = j\Delta t$. In the sequel, we use the following notations for functions $\psi, \tilde{\psi}$, which are defined on $[0,T]$ or on its division:

$$\begin{aligned} \psi_j &= \psi(t_j),\ \partial_t \psi_j = \frac{\psi_{j+1}-\psi_j}{\Delta t},\ \psi_{j+\frac12} = \frac{\psi_{j+1}+\psi_j}{2}, \\ \bar{\psi}_{j+\frac12} &= \psi(t_{j+\frac12}),\ (\psi\,\tilde{\psi})_{j+\frac12} = \psi_{j+\frac12}\,\tilde{\psi}_{j+\frac12}\,. \end{aligned} \tag{3.1}$$

Concerning the smoothness of the functions we assume

$$\begin{aligned} & u \in C^0(\widetilde{H}^1 \cap W^{2,\infty} \cap H^{r+1}),\ D_t u \in L^2(H^{r-1}),\ D_{ttt} u \in L^2(\widetilde{H}^{-1}), \\ & D_{tt} u \in L^2(H^1),\ b \in C^0(W^{1,\infty} \cap H^r)\,,\ f \in C^0(H^{r-1}) \end{aligned} \tag{3.2}$$

for $r \geq 2$. If we compare these regularity assumptions to those in (2.9) we notice some differences. The main reason for these changes is naturally the discretization in time. Especially, this brings some new assumptions concerning higher order time-derivatives of u (see the Appendix).

In order to get a totally discrete formulation, we use the well-known Crank-Nicolson scheme. We compute the discrete solution $U = U_j(b)$, which corresponds to a given parameter b, with the recursive formula

$$\left\{ \begin{aligned} (\partial_t U_j, v_h) + ((\bar{b}\,\nabla U)_{j+\frac12}, \nabla v_h) &= (\bar{f}_{j+\frac12}, v_h) \quad \forall v_h \in U_h\,, \\ U_0 &= u_{0,h}\,, \end{aligned} \right. \tag{3.3}$$

for $j = 0, ..., m-1$. Throughout this section, we use the following finite element spaces

$$U_h = S^{r,0}_{h,2},\ B_h = S^{r-1}_{h,1},\ Z_h = S^{r,0}_{h,1},\ F_h = S^{r-2}_{h,0}\,. \tag{3.4}$$

We consider first a totally discrete cost functional

$$\begin{aligned} J(b_h) &= \sum_{j=0}^{m-1} \|(\hat{U} - z_h)_{j+\frac12}\|_1^2 + h^2 \Big(\|\partial_t \hat{U}_j - \bar{\phi}_{h,j+\frac12}\|_0^2 \\ &\qquad + \|\partial_t \hat{U}_j - \nabla \cdot (\bar{\tilde{b}}_h\, \nabla \hat{U})_{j+\frac12} - \bar{f}_{h,j+\frac12}\|_0^2 \Big)\,, \end{aligned} \tag{3.5}$$

where $\hat{U} = \hat{U}_j(\tilde{b}_h)$ is calculated from (3.3) with parameter $\tilde{b}_h$, and $\bar{f}_{h,j+\frac12}$ is the interpolant of $\bar{f}_{j+\frac12}$ in F_h.

The identification problem in this totally discrete setting can be defined as:

$$\text{find } b_h \in M_h :\ J(b_h) \leq J(\tilde{b}_h) \quad \forall\, \tilde{b}_h \in M_h\,, \tag{3.6}$$

where

$$\begin{aligned} M &= \Big\{ \bar{\tilde{b}} \mid \forall\, 0 \leq j \leq m-1 :\ 0 < \lambda_1 \leq \bar{\tilde{b}}_{j+\frac12} \leq \lambda_2 < \infty \text{ a.e. in } \Omega\,, \\ &\quad \|\nabla \bar{\tilde{b}}_{j+\frac12}\|_0 \leq \mu < \infty \Big\} \end{aligned} \tag{3.7}$$

is the set for admissible parameters and $M_h = M \cap B_h$. From the definition of M_h we see that the discrete parameter is defined as a finite element function with respect to the space variables at time levels $t_{j+\frac{1}{2}}, j = 0, ..., m-1$. In the sequel, let b_h be a minimizer in (3.6) (existence follows as before) and $W = U_j(b_h)$ the solution of (3.3) with this parameter.

Again, we introduce first a few lemmas. Proofs for these results are included in the Appendix.

Lemma 3.1 *Between the true solution* $u = u(b)$ *of* (1.1) *and the discrete solution* $U = U_j(b)$ *of* (3.3) *we have an estimate*

$$\Delta t \sum_{j=0}^{m-1} \left(\|(U - \bar{u})_{j+\frac{1}{2}}\|_1^2 + \|\partial_t U_j - D_t \bar{u}_{j+\frac{1}{2}}\|_{-1}^2 \right) \leq C\,T\,(h^{2r} + (\Delta t)^4)\,. \tag{3.8}$$

Moreover, if in addition to (3.2) *we assume*

$$D_{ttt} u \in L^2(L^2),\; D_{tt} u \in L^2(H^2)\,, \tag{3.9}$$

we have an estimate

$$\Delta t \sum_{j=0}^{m-1} \left(\|(U - \bar{u})_{j+\frac{1}{2}}\|_2^2 + \|\partial_t U_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 \right) \leq C\,T\,h^{-2}(h^{2r} + (\Delta t)^4)\,. \tag{3.10}$$

Lemma 3.2 *Assume that the true parameter* b *satisfies* (2.15). *Let* θ_h *be the* L^2*-projection of* b *into* B_h *for all* $t \in [0, T]$, *and* $\widetilde{U} = \widetilde{U}_j(\theta_h)$ *the corresponding discrete solution of* (3.3). *Then, for* h *small enough,* $\theta_h \in M_h$, *and the following estimate between* $\widetilde{U}$ *and* u *holds*

$$\Delta t \sum_{j=0}^{m-1} \left(\|(\widetilde{U} - \bar{u})_{j+\frac{1}{2}}\|_1^2 + \|\partial_t \widetilde{U}_j - D_t \bar{u}_{j+\frac{1}{2}}\|_{-1}^2 \right) \leq C\,T\,(h^{2r} + (\Delta t)^4)\,.$$

If assumption (3.9) *is valid, we get an estimate*

$$\Delta t \sum_{j=0}^{m-1} \left(\|(\widetilde{U} - \bar{u})_{j+\frac{1}{2}}\|_2^2 + \|\partial_t \widetilde{U}_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 \right) \leq C\,T\,h^{-2}\,(h^{2r} + (\Delta t)^4)\,.$$

Lemma 3.3 *Assume that* b *satisfies* (2.15) *and that* (2.11) *is valid. With the smoothness assumptions* (3.2) *and* (3.9) *the following estimate between* b, u *and* b_h, W *is, for* h *small enough, valid*

$$\begin{aligned} \Delta t \sum_{j=0}^{m-1} \Big(&\|(W - \bar{u})_{j+\frac{1}{2}}\|_2^2 + \|\partial_t W_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 \\ &+ \|\partial_t W_j - \nabla \cdot (\bar{b}_h \nabla W)_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_0^2 \Big) \\ \leq C\,T\,&(h^{2(r-1)} + h^{-2}\,(\Delta t)^4 + h^{-4}\,\varepsilon_1^2 + \varepsilon_2^2)\,. \end{aligned}$$

Theorem 3.1 *Let the assumptions of Lemma 3.3 be valid. Then, for h sufficiently small, there exists a constant $C > 0$ independent of h, such that an estimate*

$$\left(\Delta t \sum_{j=0}^{m-1} \left(\int_\Omega |(\bar{b} - \bar{b}_h)_{j+\frac{1}{2}}| \, |\nabla \bar{u}_{j+\frac{1}{2}}|^2 \, dx\right)^2\right)^{\frac{1}{2}} \\ \leq CT \left(h^{r-1} + h^{-1} (\Delta t)^2 + h^{-2} \varepsilon_1 + \varepsilon_2\right)$$

between a solution b_h of (3.6) *and the true parameter b holds.*

Proof: From (1.1) we know that in $L^2(\Omega)$ an equation

$$-\nabla \cdot ((\bar{b} - \bar{b}_h) \nabla \bar{u})_{j+\frac{1}{2}} = -D_t \bar{u}_{j+\frac{1}{2}} + \bar{f}_{j+\frac{1}{2}} + \nabla \cdot (\bar{b}_h \nabla \bar{u})_{j+\frac{1}{2}} \tag{3.11}$$

is valid for all $0 \leq j \leq m-1$. Now, adding and subtracting $\partial_t W_j$ and $\nabla \cdot (\bar{b}_h \nabla W)_{j+\frac{1}{2}}$ to (3.11) we get, with the same technique as in Theorem 2.1, (2.18)

$$\int_\Omega |(\bar{b} - \bar{b}_h)_{j+\frac{1}{2}}| \, |\nabla \bar{u}_{j+\frac{1}{2}}|^2 \, dx \leq C\Big(\|\partial_t W_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0 \\ + \|(W - \bar{u})_{j+\frac{1}{2}}\|_2 + \|\partial_t W_j - \nabla \cdot (\bar{b}_h \nabla W)_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_0\Big) \tag{3.12}$$

for all $0 \leq j \leq m-1$. Hence, taking square in both sides of (3.12), summing from $j = 0, ..., m-1$, and multiplying with Δt we have

$$\Delta t \sum_{j=0}^{m-1} \left(\int_\Omega |(\bar{b} - \bar{b}_h)_{j+\frac{1}{2}}| \, |\nabla \bar{u}_{j+\frac{1}{2}}|^2 \, dx\right)^2 \\ \leq C \Delta t \sum_{j=0}^{m-1} \Big(\|\partial_t W_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 + \|(W - \bar{u})_{j+\frac{1}{2}}\|_2^2 \\ + \|\partial_t W_j - \nabla \cdot (\bar{b}_h \nabla W)_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_0^2\Big) . \tag{3.13}$$

Results from Lemma 3.3 prove the theorem.

As in the previous section, we have a better estimate for $d = 1$ with the same restrictions concerning the boundary conditions and the solution method as before. For this purpose, we define a cost functional as

$$J(b_h) = \sum_{j=0}^{m-1} \|(\hat{U} - z_h)_{j+\frac{1}{2}}\|_1^2 + \|\partial_t \hat{U}_j - \bar{\phi}_{j+\frac{1}{2}}\|_{-1}^2 \\ + \|\partial_t \hat{U}_j - (\bar{b}_h \hat{U}')'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2 . \tag{3.14}$$

Theorem 3.2 *Assume that only smoothness conditions* (3.2) *and* (2.15), (2.11) *are valid. Then, for h sufficiently small, there exists a constant $C > 0$ independent of h, such that*

$$\left(\Delta t \sum_{j=0}^{m-1} \|((\bar{b} - \bar{b}_h)\, \bar{u}')_{j+\frac{1}{2}}\|_0^2 \right)^{\frac{1}{2}} \leq CT\left(h^r + (\Delta t)^2 + h^{-1}\,\varepsilon_1 + \varepsilon_2\right) ,$$

where b_h is a minimizer of (3.14).

Proof: With the same technique as in Theorem 2.2, (2.23), and in (3.11), (3.12) we get

$$\begin{aligned} \|((\bar{b} - \bar{b}_h)\bar{u}')_{j+\frac{1}{2}}\|_0 \quad &\leq C\Big(\|\partial_t W_j - D_t \bar{u}_{j+\frac{1}{2}}\|_{-1} + \|(W - \bar{u})'_{j+\frac{1}{2}}\|_0 \\ &\quad + \|\partial_t W_j - (\bar{b}_h\, W')'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}\Big) \end{aligned} \tag{3.15}$$

for all $0 \leq j \leq m-1$. As in the previous theorem, it follows from (3.15)

$$\begin{aligned} &\Delta t \sum_{j=0}^{m-1} \|((\bar{b} - \bar{b}_h)\bar{u}')_{j+\frac{1}{2}}\|_0^2 \\ &\leq C\Delta t \sum_{j=0}^{m-1} \Big(\|\partial_t W_j - D_t \bar{u}_{j+\frac{1}{2}}\|_{-1}^2 + \|(W - \bar{u})_{j+\frac{1}{2}}\|_1^2 \\ &\qquad + \|\partial_t W_j - (\bar{b}_h\, W')'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2\Big) . \end{aligned} \tag{3.16}$$

As in the proof of Lemma 3.3 when using again the results from Lemma 3.2, we can show that the cost functional (3.14) satisfies an estimate

$$\begin{aligned} &\Delta t \sum_{j=0}^{m-1} \|(W - z_h)_{j+\frac{1}{2}}\|_1^2 + \|\partial_t W_j - \bar{\phi}_{h,j+\frac{1}{2}}\|_{-1}^2 \\ &\qquad + \|\partial_t W_j - (\bar{b}_h\, W')'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2 \\ &\leq CT(h^{2r} + (\Delta t)^4 + h^{-2}\,\varepsilon_1^2 + \varepsilon_2^2) . \end{aligned} \tag{3.17}$$

As before, the result follows from (3.17).

Remark 3.1 It is clear that in the semidiscrete case we can not remove the assumption about the existence of an observation for $D_t u$. However, because we assumed that the observation of u is of the form $z_j = z(t_j)$, one (simplest) possibility is to approximate $\bar{\phi}_{h,j+\frac{1}{2}}$ with $\partial_t z_{h,j}$, $j = 0, ..., m-1$. A similar analysis as before shows that for a cost functional

$$\begin{aligned} J(b_h) \quad &= \sum_{j=0}^{m-1} \|(\hat{U} - z_h)_{j+\frac{1}{2}}\|_1^2 + (\Delta t)^2\, \|\partial_t \hat{U}_j - \partial_t z_{h,j}\|_0^2 \\ &\qquad + h^2 \|\partial_t \hat{U}_j - \nabla \cdot (\tilde{\bar{b}}_h\, \nabla \hat{U})_{j+\frac{1}{2}} - \bar{f}_{h,j+\frac{1}{2}}\|_0^2 , \end{aligned} \tag{3.18}$$

the result of Theorem 3.1 is replaced with an estimate

$$\begin{aligned} &\left(\Delta t \sum_{j=0}^{m-1} \left(\int_\Omega |(\bar{b}-\bar{b}_h)_{j+\frac{1}{2}}|\,|\nabla \bar{u}_{j+\frac{1}{2}}|^2\,dx\right)^2\right)^{\frac{1}{2}} \\ &\le CT\left(h^{r-1} + (\Delta t)^{-1}h^r + h^{-1}(\Delta t)^2 + \Delta t + h^{-1}(h^{-1}+(\Delta t)^{-1})\,\varepsilon_1\right). \end{aligned} \tag{3.19}$$

For $d=1$, a minimization of a cost functional

$$\begin{aligned} J(b_h) \;&= \sum_{j=0}^{m-1} \|(\hat{U}-z_h)_{j+\frac{1}{2}}\|_1^2 + (\Delta t)^2 \|\partial_t \hat{U}_j - \partial_t z_{h,j}\|_{-1}^2 \\ &\quad + \|\partial_t \hat{U}_j - (\bar{b}_h\,\hat{U}')'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2 \end{aligned} \tag{3.20}$$

gives an estimate

$$\begin{aligned} &\left(\Delta t \sum_{j=0}^{m-1} \|((\bar{b}-\bar{b}_h)\,\bar{u}')_{j+\frac{1}{2}}\|_0^2\right)^{\frac{1}{2}} \\ &\le CT\left((\Delta t)^{-1}h^r + \Delta t + (h^{-1}+(\Delta t)^{-1})\,\varepsilon_1\right) \end{aligned} \tag{3.21}$$

as a replacement of Theorem 3.2. Notice that we can also replace $\bar{f}_{h,j+\frac{1}{2}}$ with $f_{h,j+\frac{1}{2}}$, if $D_{tt}f \in L^2(L^2)$ with the first cost functional (3.18), or $D_{tt}f \in L^2(\widetilde{H}^{-1})$ with the cost functional (3.20).

Remark 3.2 If $m(\,,{}_0) > 0$, we can replace $\|(\hat{U}-\bar{z}_h)_{j+\frac{1}{2}}\|_1^2$ with $\|\nabla(\hat{U}-\bar{z}_h)_{j+\frac{1}{2}}\|_0^2$ in all cost functionals. This follows from the Poincare inequality.

Lemma 3.4 *Calculation of the dual norm. Suppose that we need to compute the $\widetilde{H}^{-1}$-norm of a given function g (notice that with the proposed methods this calculation needs to be done only on fixed time levels). Then $\|g\|_{-1}$ is equal to $\|\varphi\|_1$ where φ is the weak Galerkin solution of the problem*

$$\begin{cases} -\Delta\varphi + \varphi &= g \text{ in } \Omega\,, \\ \varphi|_{,\,0} = \left.\dfrac{\partial\varphi}{\partial n}\right|_{,\,1} &= 0\,. \end{cases} \tag{3.22}$$

Proof: A direct calculation using the definition of the dual norm and (2.8), (5.2).

Remark 3.3 *In Lemma 3.4 we can replace $-\Delta\varphi+\varphi = g$ with $-\Delta\varphi = g$, if $m(\,,{}_0) > 0$. Then we have an equivalence between $\|\nabla\varphi\|_0$ and $\|g\|_{-1}$. This follows again from the Poincare inequality.*

4 Numerical Experiments

Since we gave improved estimates for the $1d$ case in the previous section, this is the result we will investigate. Moreover, even if this is not along with our theory, these results are computed using only a C^0 finite element space in U_h. In this way, there are fewer degrees of freedom to optimize with respect to u. Moreover, in practical applications this is surely a more flexible choice, and it is also very interesting to see what will happen and is there a possibility to improve the theoretical results in this respect. We will see that the answer to this last question is yes.

As we mentioned in the introduction, all error estimates given remain valid when we treat b and u as separate variables in the cost functional. Moreover, computationally this is much easier, since the gradients with respect to the variables can be calculated directly without solving any adjoint equations. Therefore, for $(t,x) \in (0,1) \times (0,1)$, we minimize a cost functional

$$\begin{aligned} J(u_h, b_h) &= \sum_{j=0}^{m-1} \|(u_h - z_h)'_{j+\frac{1}{2}}\|_0^2 + \|\partial_t u_{h,j} - \bar{\phi}_{j+\frac{1}{2}}\|_{-1}^2 \\ &\qquad + \|\partial_t u_{h,j} - (\bar{b}_h\, u'_h)'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2 \end{aligned} \tag{4.1}$$

over $U_h \times M_h$. Here, $U_h \subset \widetilde{H}^1 = \{v \in H^1 \mid v(0) = 0\}$, and the set of admissible parameters is of the form

$$\begin{aligned} M_h &= \Big\{ \bar{b}_h \in (B_h)^m \,|\, \forall\, 0 \le j \le m-1 :\, 0 < \lambda_1 \le \bar{b}_{h,j+\frac{1}{2}} \le \lambda_2 < \infty\,, \\ &\qquad \|\bar{b}'_{h,j+\frac{1}{2}}\|_0 \le \mu < \infty \Big\}\,. \end{aligned} \tag{4.2}$$

Throughout this section, we choose $U_h = S^2_{h,1}$ and $B_h = S^1_{h,1}$, i.e., we use a piecewise quadratic Lagrange basis in U_h and a corresponding linear basis in B_h.

The minimization of (4.1) was made using the following sequential splitting algorithm (compare to the augmented Lagrangian algorithm in [13]):

Sequential splitting algorithm

1. Initialize $k = 0$, $u_0 = u_{h,0} = z_h$.
2. For given u_k,

$$\min_{b_k \in M_h} J(b_k) = \sum_{j=0}^{m-1} \|\partial_t u_{k,j} - (\bar{b}_k\, u'_k)'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2. \tag{4.3}$$

3. For given b_k,

$$\min_{u_{k+1}} J(u_{k+1}) = \sum_{j=0}^{m-1} \|(u_{k+1} - z_h)'_{j+\frac{1}{2}}\|_0^2 + \|\partial_t u_{k+1,j} - \bar{\phi}_{j+\frac{1}{2}}\|_{-1}^2 + \|\partial_t u_{k+1,j} - (\bar{b}_k\, u'_{k+1})'_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_{-1}^2. \quad (4.4)$$

4. Test the convergence. Stop or set $k = k+1$ and goto 2 .

In the actual computations, each subproblem in the algorithm was solved using the E04UCF optimization routine from the NAG-library. In all examples, $b(t,x) = \exp(t)\exp(x)$ and $u(t,x) = \exp(-t)\sin(\pi x)^2$.

Example 4.1 First we study the relation between Δt and h. We fix $\Delta t = \frac{1}{6}$ and vary h. Observations are assumed to be exact in this example.

$\frac{1}{h}$	error	iterations
3	$5.047 \cdot 10^{-2}$	19
4	$2.836 \cdot 10^{-2}$	20
5	$1.883 \cdot 10^{-2}$	6
6	$1.570 \cdot 10^{-2}$	3
7	$1.465 \cdot 10^{-2}$	2
8	$1.417 \cdot 10^{-2}$	2
9	$1.392 \cdot 10^{-2}$	2
10	$1.378 \cdot 10^{-2}$	2
11	$1.369 \cdot 10^{-2}$	2
12	$1.364 \cdot 10^{-2}$	3
18	$1.354 \cdot 10^{-2}$	3

Table 1: Calculated results in Example 4.1 with different values of h.

Since after $h = \frac{1}{6}$ the magnitude of error decreasing gets clearly smaller, and after $h = \frac{1}{10}$ the error remains practically the same, $\Delta t \sim h$ (up to a constant) seems to be the best choice. Moreover, the number of iterations taken by the algorithm indicates the same balance.

Example 4.2 Same as the first example, but we take $\Delta t = h$ and test the order of convergence.

$\frac{1}{h}$	error	error/h^2
3	$7.793 \cdot 10^{-2}$	0.701
4	$4.084 \cdot 10^{-2}$	0.653
5	$2.406 \cdot 10^{-2}$	0.602
6	$1.570 \cdot 10^{-2}$	0.565
7	$1.120 \cdot 10^{-2}$	0.549
8	$8.419 \cdot 10^{-3}$	0.538
9	$6.573 \cdot 10^{-3}$	0.532
10	$5.277 \cdot 10^{-3}$	0.528
11	$4.334 \cdot 10^{-3}$	0.524
12	$3.624 \cdot 10^{-3}$	0.522

Table 2: Calculated results in Example 4.2 with different values of h.

Table 2 confirms the $O(h^2 + \Delta t^2)$ rate of convergence.

Example 4.3 As Example 4.2, but with an observation error $z_h(x_i) = u(x_i) + \varepsilon(x_i)$ in the discretization points x_i for all t. Here $\varepsilon_1 = \|u - z_h\|_0 = 0.001$ and

$$\varepsilon(x) = \begin{cases} -\varepsilon_1, \quad 0 \le x < \frac{1}{4}, \ \frac{1}{2} \le x < \frac{3}{4}, \\ \varepsilon_1, \text{ elsewhere.} \end{cases} \tag{4.5}$$

We expect an error of the form $C_1 h^2 + C_2 \frac{\varepsilon_1}{h}$. We can get $C_1 h^2$ -term from Table 2, since it represents the error with perfect observation. Therefore, in the third column of the next table, we have calculated $C_2 = \frac{h}{\varepsilon_1}(\text{error} - C_1 h^2)$.

$\frac{1}{h}$	error	C_2
3	$7.657 \cdot 10^{-2}$	-
4	$4.705 \cdot 10^{-2}$	1.552
5	$2.751 \cdot 10^{-2}$	0.689
6	$2.818 \cdot 10^{-2}$	2.079
7	$2.762 \cdot 10^{-2}$	2.345
8	$3.061 \cdot 10^{-2}$	2.774
9	$3.077 \cdot 10^{-2}$	2.689
10	$3.502 \cdot 10^{-2}$	2.974
11	$3.336 \cdot 10^{-2}$	2.639
12	$3.825 \cdot 10^{-2}$	2.886

Table 3: Calculated results in Example 4.3 with different values of h.

The constant C_2 seems to get stabilized. The "zig-zag" phenomena in this and the previous tables is due to the location of the difficult points $u' = 0$ with respect to the element division of the interval $(0,1)$. The most important information in Table 3 is clearly the fact that with the observation error, decreasing h increases the error for h small enough. This is a very important matter in practice, where one should be able to improve the observation and not just make h smaller to get better results.

Remark 4.1 We computed the given examples with homogenous Dirichlet boundary conditions as well. The obtained results were exactly of the same form as for the mixed problem. Therefore, it should be possible to prove corresponding error estimates as well. However, at the moment this is theoretically still an open question.

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5 Appendix

In fact, many of the results included in this Appendix can be proved using standard techniques (see, for example, [1] and articles therein). However, to use standard methods here is not the best way from the point of view of parameter identification. Since the parameter function $b(t,x)$ in the original equation (1.1) is usually not the main issue, it is assumed to be "smooth enough", which in parameter identification is not the case. One important aspect is the regularity of different parameters appearing in the equation. This is the reason, why we have tried to establish the following results under minimal assumptions for the parameters, and therefore, some parts are not standard.

For completeness, let us recall the interpolation properties of the spaces $S^r_{h,l}$ (see, e.g., [1]): for all $v \in W^{m,p}(\Omega) \subset C^{l-1}(\bar{\Omega})$ there exists an interpolant $I_h v \in S^r_{h,l}$ such that

$$\|v - I_h v\|_{k,p} \leq C h^{m-k} \|v\|_{m,p} \quad \text{for} \quad 0 \leq k \leq l,\ m \leq r+1,\ 1 \leq p \leq \infty\,. \tag{5.1}$$

In many places, we make use of the following inequality:

Let $a, b \in \mathbb{R}$. Then, for $\alpha > 0$,

$$a\,b \leq \frac{1}{4\,\alpha} a^2 + \alpha b^2\,. \tag{5.2}$$

5.1 Proofs of lemmas in section 2

Proof of Lemma 2.1: Because $U_h \subset \widetilde{H}^1$, subtracting (2.4) from (2.2) leads to a formula

$$(D_t(u_h - u), v_h) + (b\,\nabla(u_h - u), \nabla v_h) = 0 \quad \forall v_h \in U_h\,. \tag{5.3}$$

Let $\bar{u}_h$ be an arbitrary element in U_h. Then, (5.3) can be also written as

$$\begin{aligned}&(D_t(u_h - \bar{u}_h), v_h) + (b\,\nabla(u_h - \bar{u}_h), \nabla v_h)\\ &= (D_t(u - \bar{u}_h), v_h) + (b\,\nabla(u - \bar{u}_h), \nabla v_h) \quad \forall v_h \in U_h\,.\end{aligned} \tag{5.4}$$

Let $P_h w$ be the H^1-projection of w into U_h, i.e.,

$$(w - P_h w, v_h) + (\nabla(w - P_h w), \nabla v_h) = 0 \quad \forall v_h \in U_h\,. \tag{5.5}$$

By the definition, $P_h w$ is stable in H^1

$$\|P_h w\|_1 \le \|w\|_1 \quad \forall w \in H^1\,. \tag{5.6}$$

Let $\psi \in \widetilde{H}^1$ be given, and define φ as the solution of the problem

$$\begin{cases} -\Delta\varphi + \varphi &= \psi \text{ in } \Omega,\\ \left.\dfrac{\partial\varphi}{\partial n}\right|_{\partial\Omega} &= 0. \end{cases} \tag{5.7}$$

By standard regularity results we have $\|\varphi\|_3 \le C\,\|\psi\|_1$, which by Sobolev imbedding theorem means that $\varphi \in C^1(\bar{\Omega})$ for $d \le 3$. Then, using (5.7), (5.5), and (5.1) we have

$$\begin{aligned}(w - P_h w, \psi) &= (w - P_h w, \varphi) + (\nabla(w - P_h w), \nabla\varphi)\\ &= (w - P_h w, \varphi - I_h\varphi) + (\nabla(w - P_h w), \nabla(\varphi - I_h\varphi))\\ &\le C\,\|w - P_h w\|_1\,h^2\|\varphi\|_3 \le C\,\|w - P_h w\|_1\,h^2\|\psi\|_1.\end{aligned} \tag{5.8}$$

Hence, this gives

$$\|w - P_h w\|_{-1} = \sup_{\psi\in\widetilde{H}^1} \frac{|(w - P_h w, \psi)|}{\|\psi\|_1} \le C\,h^2\,\|w - P_h w\|_1 \le C\,h^2\,\|w\|_1\,, \tag{5.9}$$

and so

$$\begin{aligned}\|w - P_h w\|_0^2 &\le \|w - P_h w\|_{-1}\,\|w - P_h w\|_1 \le C\,h^2\|w - P_h w\|_1^2\\ &\le C\,h^2\,\|w\|_1^2\,.\end{aligned} \tag{5.10}$$

For fixed $t \in [0,T]$, let $\bar{u}_h(t)$ be the L^2-projection of $u(t)$ into U_h, i.e.,

$$(u(t) - \bar{u}_h(t), v_h) = 0 \quad \forall v_h \in U_h \,. \tag{5.11}$$

Again, it follows that this projection is stable in L^2

$$\|\bar{u}_h(t)\|_0 \le \|u(t)\|_0 \quad \forall u(t) \in L^2 \,, \tag{5.12}$$

and that we have an abstract approximation result

$$\|u(t) - \bar{u}_h(t)\|_0 = \inf_{\chi \in U_h} \|u(t) - \chi\|_0 \,. \tag{5.13}$$

From (5.1) we obtain for all $u \in H^m(\Omega) \subset C^1(\bar{\Omega})$ $(m > 1 + \frac{d}{2})$

$$\|u(t) - \bar{u}_h(t)\|_0 \le C\, h^s \, \|u(t)\|_s, \quad m \le s \le r+2 \,. \tag{5.14}$$

But, from (5.10) and (5.13) it follows that also

$$\|u(t) - \bar{u}_h(t)\|_0 \le C\, h \, \|u\|_1 \,. \tag{5.15}$$

Hence, by interpolation (see, e.g., [10], Lemma 7) we get

$$\|u(t) - \bar{u}_h(t)\|_0 \le C\, h^s \, \|u(t)\|_s, \quad 1 \le s \le r+2 \,. \tag{5.16}$$

Moreover, using the standard inverse inequalities one obtains from (5.16) error estimates with respect to higher order norms. Finally, using (5.11) and (5.10)

$$\begin{aligned} &(u(t) - \bar{u}_h(t), \psi) = \\ &\qquad (u(t) - \bar{u}_h(t), \psi - P_h\psi) \le C\, \|u(t) - \bar{u}_h(t)\|_0 \, h \, \|\psi\|_1 \\ &\qquad \forall \psi \in \widetilde{H}^1 \,. \end{aligned} \tag{5.17}$$

This improves the order of convergence with respect to the dual norm $\|\cdot\|_{-1}$ by one. Notice here that another way of deriving the estimates needed is to apply directly Theorem 12.4.2 in [4] (where it is taken from [5]) to (5.13).

By differentiating (5.11) with respect to t we find

$$\frac{d}{dt}(u(t) - \bar{u}_h(t), v_h) = (D_t(u(t) - \bar{u}_h(t)), v_h) = 0 \quad \forall v_h \in U_h \,, \tag{5.18}$$

which means that the L^2-projection commutes with time differentiation. This implies as before that estimates

$$\|D_t(u(t) - \bar{u}_h(t))\|_k \le C\, h^{r-1-k} \, \|D_t u(t)\|_{r-1}, \quad -1 \le k \le 1 \,, \tag{5.19}$$

are also valid.

For simplicity, we denote from now on all functions without t. Taking into account (5.18) in (5.4) leads to a formula

$$(D_t(u_h - \bar{u}_h), v_h) + (b\,\nabla(u_h - \bar{u}_h), \nabla v_h) = (b\,\nabla(u - \bar{u}_h), \nabla v_h) \quad \forall v_h \in U_h\,. \tag{5.20}$$

Now we choose $v_h = u_h - \bar{u}_h$ in (5.20). Using (2.15) and (5.2) it follows

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|u_h - \bar{u}_h\|_0^2 \quad &+ \quad \lambda_1 \|\nabla(u_h - \bar{u}_h)\|_0^2 \\ &\le \quad \frac{1}{4\alpha}\lambda_2^2\,\|\nabla(u - \bar{u}_h)\|_0^2 + \alpha\|\nabla(u_h - \bar{u}_h)\|_0^2\,. \end{aligned} \tag{5.21}$$

An integration over $(0,t)$ for $0 < t \le T$ and the choice $\alpha < \lambda_1$ gives

$$\begin{aligned} &\|u_h - \bar{u}_h\|_0^2 + \int_0^t \|u_h - \bar{u}_h\|_1^2\,ds \\ &\le \|u_{0,h} - \bar{u}_{0,h}\|_0^2 + C\int_0^t \|\nabla(u - \bar{u}_h)\|_0^2\,ds + \int_0^t \|u_h - \bar{u}_h\|_0^2\,ds \\ &\le \|u_{0,h} - \bar{u}_{0,h}\|_0^2 + C\,h^{2(r+1)}\,\|u\|_{L^2(H^{r+2})}^2 + \int_0^t \|u_h - \bar{u}_h\|_0^2\,ds\,, \end{aligned} \tag{5.22}$$

where $\int_0^t \|u_h - \bar{u}_h\|_0^2\,ds$ was added to both sides. For the first term on the right-hand side we have

$$\|u_{0,h} - \bar{u}_{0,h}\|_0 \le \|u_{0,h} - u_0\|_0 + \|u_0 - \bar{u}_{0,h}\|_0 \le C\,h^{r+1}\,\|u_0\|_{r+1}\,. \tag{5.23}$$

Thus, (5.16), (5.22), (5.23), and an application of Gronwall's inequality give

$$\begin{aligned} \|u - u_h\|_{C^0(L^2)} &\le \|u - \bar{u}_h\|_{C^0(L^2)} + \|\bar{u}_h - u_h\|_{C^0(L^2)} \\ &\le C\,h^{r+1}\,(\|u_0\|_{r+1} + \|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})}) \\ &\le C\,h^{r+1}\,(\|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})})\,, \end{aligned} \tag{5.24}$$

which proves the L^2-estimate. Similarly, from the second term in (5.22) we find that estimate

$$\|u - u_h\|_{L^2(H^1)} \le C\,h^{r+1}\,(\|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})}) \tag{5.25}$$

is also correct. Moreover, using the inverse inequality

$$\|\chi\|_1 \le Ch^{-1}\|\chi\|_0 \;\forall \chi \in U_h,$$

it follows from (5.24)

$$\begin{aligned}\|u-u_h\|_{C^0(H^1)} &\le \|u-I_hu\|_{C^0(H^1)} + C\,h^{-1}\,\|I_hu-u_h\|_{C^0(L^2)} \\ &\le C\,h^r\,\|u\|_{C^0(H^{r+1})} + C\,h^{-1}\,(\|I_hu-u\|_{C^0(L^2)} \\ &\quad +\|u-u_h\|_{C^0(L^2)}) \\ &\le C\,h^r\,(\|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})})\,. \end{aligned} \tag{5.26}$$

Let $\psi_h \in U_h$ be the L^2-projection of a given $\psi \in \widetilde{H}^1$. Then, using the inverse inequality again, (5.10), and (5.16) we can show that

$$\|\psi_h\|_1 \le C\,\|\psi\|_1\,. \tag{5.27}$$

Therefore, by the definition of the L^2-projection and using (5.20) we get

$$\begin{aligned}&\|D_t(u_h-\bar{u}_h)\|_{-1} = \\ &\quad \sup_{\psi\in\widetilde{H}^1}\frac{|(D_t(u_h-\bar{u}_h),\psi)|}{\|\psi\|_1} = \sup_{\psi\in\widetilde{H}^1}\frac{|(D_t(u_h-\bar{u}_h),\psi_h)|}{\|\psi\|_1} \\ &\quad \le \sup_{\psi\in\widetilde{H}^1}\frac{|(b\,\nabla(u_h-\bar{u}_h),\nabla\psi_h)| + |(b\,\nabla(u-\bar{u}_h),\nabla\psi_h)|}{\|\psi\|_1} \\ &\quad \le C\,(\|\nabla(u_h-\bar{u}_h)\|_0 + \|\nabla(u-\bar{u}_h)\|_0) \\ &\quad \le C\,h^r\,(\|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})}) \quad \forall t\in[0,T]\,. \end{aligned} \tag{5.28}$$

This and (5.19) prove the third estimate. With the duality technique a similar calculation as in (5.28), when using again the inverse inequality, (5.12), and the fact $\psi_h \in U_h \subset H^1$, shows

$$\begin{aligned}&\|D_t(u_h-\bar{u}_h)\|_0 = \\ &\quad \sup_{\psi\in L^2}\frac{|(D_t(u_h-\bar{u}_h),\psi)|}{\|\psi\|_0} = \sup_{\psi\in L^2}\frac{|(D_t(u_h-\bar{u}_h),\psi_h)|}{\|\psi\|_0} \\ &\quad \le \sup_{\psi\in L^2}\frac{(\|b\,\nabla(u_h-\bar{u}_h)\|_0 + \|b\,\nabla(u-\bar{u}_h)\|_0)\,C\,h^{-1}\,\|\psi_h\|_0}{\|\psi\|_0} \\ &\quad \le C\,h^{-1}\,(\|\nabla(u_h-\bar{u}_h)\|_0 + \|\nabla(u-\bar{u}_h)\|_0) \\ &\quad \le C\,h^{r-1}\,(\|u\|_{C^0(H^{r+1})} + \|u\|_{L^2(H^{r+2})}) \quad \forall t\in[0,T]\,. \end{aligned} \tag{5.29}$$

Hence, (5.29) combined with (5.19) proves the last result in the lemma.

Proof of Lemma 2.2: Between $b = b(t)$ and $\theta_h = \theta_h(t)$ we have, $\forall t \in [0,T]$, the following estimates which can be shown as in Lemma 2.1

$$\begin{aligned}\|b-\theta_h\|_k &\le C\,h^{s-k}\,\|b\|_s, \quad 0\le k\le 1,\ k\le s\le r+1\,, \\ \|b-\theta_h\|_{k,\infty} &\le C\,h^{1-k}\,\|b\|_{1,\infty},\ 0\le k\le 1\,. \end{aligned} \tag{5.30}$$

(2.15) means that there exists a positive constant $\delta > 0$ such that $\forall t \in [0,T]$:

$$\begin{aligned} &\lambda_1 + \delta \le b \le \lambda_2 - \delta \text{ a.e in } \Omega\,, \\ &\|\nabla b\|_0 \le \mu - \delta\,. \end{aligned} \tag{5.31}$$

Hence, it follows from (5.30) and (5.31)

$$\|\nabla\theta_h\|_0 \le \|\nabla(\theta_h - b)\|_0 + \|\nabla b\|_0 \le C\,h\,\|b\|_2 + \mu - \delta \le \mu \tag{5.32}$$

for h small enough. Similarly we see that, for h small enough, θ_h satisfies

$$\begin{aligned} &\lambda_1 \le \theta_h \le \lambda_2 \text{ a.e. in } \Omega\,, \\ &\|\nabla\theta_h\|_0 \le \mu\,, \\ &\|\theta_h\|_{1,\infty} \le C\,\|b\|_{1,\infty} \le C \end{aligned} \tag{5.33}$$

$\forall t \in [0,T]$, so $\theta_h \in M_h$ for h small enough.

From (2.4) we know that $u_h(\theta_h)$ is the solution of

$$\begin{aligned} (D_t u_h(\theta_h), v_h) + (\theta_h\,\nabla u_h(\theta_h), \nabla v_h) &= (f, v_h) \quad \forall v_h \in U_h\,, \\ u_h(\theta_h)(0,x) &= u_{0,h} \quad \text{in } \Omega\,. \end{aligned} \tag{5.34}$$

Subtracting (2.4) from (5.34) gives

$$\left\{ \begin{aligned} &(D_t(u_h(\theta_h) - u_h), v_h) + (\theta_h\,\nabla(u_h(\theta_h) - u_h), \nabla v_h) \\ &= (f, v_h) - (D_t u_h, v_h) - (\theta_h\,\nabla u_h, \nabla v_h) \\ &= (D_t u_h, v_h) + (b\,\nabla u_h, \nabla v_h) - (D_t u_h, v_h) - (\theta_h\,\nabla u_h, \nabla v_h) \\ &= ((b - \theta_h)\,\nabla u_h, \nabla v_h) \\ &= ((b - \theta_h)\,\nabla(u_h - u), \nabla v_h) + ((b - \theta_h)\,\nabla u, \nabla v_h) \quad \forall v_h \in U_h\,, \\ &[u_h(\theta_h) - u_h]|_{\Gamma_0} = 0\,, \\ &u_{0,h}(\theta_h) - u_{0,h} = 0\,. \end{aligned} \right. \tag{5.35}$$

In the sequel, we denote by $g_h = u_h(\theta_h) - u_h$. Let us first choose $v_h = g_h$ in (5.35). As in (5.21) we get, using (5.33), (5.2), and (5.30)

$$\frac{1}{2}\frac{d}{dt}\|g_h\|_0^2 + \lambda_1\|\nabla g_h\|_0^2 \le C\,(\|\nabla(u_h - u)\|_0^2 + \|b - \theta_h\|_0^2) + \alpha\,\|\nabla g_h\|_0^2\,. \tag{5.36}$$

Take $\alpha < \lambda_1$. Since $g_h = 0$ for $t = 0$, it follows from (5.36), Lemma 2.1, and (5.30)

$$\begin{aligned} \|g_h\|_0^2 + \int_0^t \|\nabla g_h\|_0^2\,ds &\le C\,(\|u_h - u\|_{L^2(H^1)}^2 + \|b - \theta_h\|_{L^2(L^2)}^2) \\ &\le C\,h^{2(r+1)}\,. \end{aligned} \tag{5.37}$$

Thus, using Lemma 2.1 once more we obtain

$$\|u_h(\theta_h) - u\|_{C^0(L^2)} \le \|g_h\|_{C^0(L^2)} + \|u_h - u\|_{C^0(L^2)} \le C\, h^{r+1} \,. \tag{5.38}$$

Exactly as in (5.26) it follows from (5.38)

$$\|u_h(\theta_h) - u\|_{C^0(H^1)} \le C\, h^r \,, \tag{5.39}$$

which proves the first part of the lemma.

Using the equation (5.35) we deduce as in (5.28)

$$\begin{aligned}
&\|D_t g_h\|_{-1} = \sup_{\psi \in \tilde{H}^1} \frac{|(D_t g_h, \psi)|}{\|\psi\|_1} = \sup_{\psi \in \tilde{H}^1} \frac{|(D_t g_h, \psi_h)|}{\|\psi\|_1} \\
&= \sup_{\psi \in \tilde{H}^1} \frac{|(-\theta_h \nabla g_h + (b-\theta_h)\nabla(u_h - u) + (b-\theta_h)\nabla u, \nabla \psi_h)|}{\|\psi\|_1} \\
&\le C\,(\|\nabla g_h\|_0 + \|\nabla(u_h - u)\|_0 + \|b - \theta_h\|_0) \\
&\le C\, h^r \quad \forall t \in [0,T] \,,
\end{aligned} \tag{5.40}$$

where the final estimate follows from (5.39), Lemma 2.1, and (5.30). Moreover, like in (5.29), we can show that the estimate $O(h^{r-1})$ is valid for $D_t g_h$ in L^2 $\forall t \in [0,T]$. This ends the proof.

Proof of Lemma 2.3: Because b_h is a minimizer of (2.12) and because, for h small enough, also $\theta_h \in M_h$, we have $\forall t \in [0,T]$:

$$\begin{aligned}
&\|w_h - z_h\|_0^2 + h^4\left(\|D_t w_h - \phi_h\|_0^2 + \|D_t w_h - \nabla\cdot(b_h \nabla w_h) - f_h\|_0^2\right) \\
&\le \|u_h(\theta_h) - z_h\|_0^2 \\
&+ h^4\left(\|D_t u_h(\theta_h) - \phi_h\|_0^2 + \|D_t u_h(\theta_h) - \nabla\cdot(\theta_h \nabla u_h(\theta_h)) - f_h\|_0^2\right) \\
&= I_1 + h^4\,(I_2 + I_3) \ ,
\end{aligned} \tag{5.41}$$

where we have denoted

$$\begin{aligned}
I_1 &= \|u_h(\theta_h) - z_h\|_0^2 \,, \\
I_2 &= \|D_t u_h(\theta_h) - \phi_h\|_0^2 \,, \\
I_3 &= \|D_t u_h(\theta_h) - \nabla\cdot(\theta_h \nabla u_h(\theta_h)) - f_h\|_0^2 \,.
\end{aligned} \tag{5.42}$$

For I_1 we have, by (2.11) and Lemma 2.2

$$I_1 \le 2\,(\|u_h(\theta_h) - u\|_0^2 + \|u - z_h\|_0^2) \le C\,(h^{2(r+1)} + \varepsilon_1^2) \,. \tag{5.43}$$

Similarly, for I_2

$$I_2 \le 2\,(\|D_t(u_h(\theta_h) - u)\|_0^2 + \|D_t u - \phi_h\|_0^2) \le C\,(h^{2(r-1)} + \varepsilon_2^2) \,. \tag{5.44}$$

Using the regularity of f and u, (1.1), and (5.33) it follows

$$
\begin{aligned}
I_3 &\le 2\,(\|D_t u_h(\theta_h) - \nabla\cdot(\theta_h\,\nabla u_h(\theta_h)) - f\|_0^2 + \|f - f_h\|_0^2) \\
&\le 2\,(\|D_t u_h(\theta_h) - \nabla\cdot(\theta_h\,\nabla u_h(\theta_h)) - D_t u + \nabla\cdot(b\,\nabla u)\|_0^2) + C\,h^{2(r-1)} \\
&\le C\,(\|D_t(u_h(\theta_h) - u)\|_0^2 + \|\nabla\cdot((b-\theta_h)\,\nabla u)\|_0^2 \\
&+\|\nabla\cdot(\theta_h\,\nabla(u - u_h(\theta_h)))\|_0^2 + h^{2(r-1)}) \\
&\le C\,(\|D_t(u_h(\theta_h) - u)\|_0^2 + \|\theta_h - b\|_1^2 + \|u_h(\theta_h) - u\|_2^2 + h^{2(r-1)})\,.
\end{aligned}
\tag{5.45}
$$

Lemma 2.2 bounds the first term and (5.30) the second term with $O(h^{2(r-1)})$. Using the inverse inequality, (5.1), and again Lemma 2.2 we get

$$
\begin{aligned}
\|u_h(\theta_h) - u\|_2 &\le C\,h^{-2}\,\|u_h(\theta_h) - I_h u\|_0 + \|I_h u - u\|_2 \\
&\le C\,h^{-2}\,\|u_h(\theta_h) - u\|_0 + C\,h^{r-1} \\
&\le C\,h^{r-1}\,.
\end{aligned}
\tag{5.46}
$$

A combination of (5.41) - (5.46) leads to

$$
\begin{aligned}
&\|w_h - z_h\|_0^2 + h^4\left(\|D_t w_h - \phi_h\|_0^2 + \|D_t w_h - \nabla\cdot(b_h\,\nabla w_h) - f_h\|_0^2\right) \\
&\le C\,(h^{2(r+1)} + \varepsilon_1^2 + h^4\,\varepsilon_2^2) \quad \forall t \in [0,T]\,.
\end{aligned}
\tag{5.47}
$$

Thus, from (5.47) we obtain estimates

$$
\begin{aligned}
\|w_h - z_h\|_{C^0(L^2)} &\le C\,(h^{r+1} + \varepsilon_1 + h^2\,\varepsilon_2)\,, \\
\|D_t w_h - \phi_h\|_{C^0(L^2)} &\le C\,(h^{r-1} + h^{-2}\,\varepsilon_1 + \varepsilon_2)\,, \\
\|D_t w_h - \nabla\cdot(b_h\,\nabla w_h) - f_h\|_{C^0(L^2)} &\le C\,(h^{r-1} + h^{-2}\varepsilon_1 + \varepsilon_2)\,.
\end{aligned}
\tag{5.48}
$$

From these estimates we deduce, exactly as in the analysis of $I_1 - I_3$,

$$
\begin{aligned}
\|w_h - u\|_{C^0(L^2)} &\le C\,(h^{r+1} + \varepsilon_1 + h^2\,\varepsilon_2)\,, \\
\|D_t(w_h - u)\|_{C^0(L^2)} &\le C\,(h^{r-1} + h^{-2}\,\varepsilon_1 + \varepsilon_2)\,, \\
\|D_t w_h - \nabla\cdot(b_h\,\nabla w_h) - f\|_{C^0(L^2)} &\le C\,(h^{r-1} + h^{-2}\varepsilon_1 + \varepsilon_2)\,.
\end{aligned}
\tag{5.49}
$$

As in (5.46) we can show, starting from the first estimate in (5.49) that between w_h and u the estimates in $C^0(H^1)$ and $C^0(H^2)$ are correct. This ends the proof.

5.2 Proofs of lemmas in section 3

Proof of Lemma 3.1: From (2.4) and $U_h \subset \widetilde{H}^1$ it follows that

$$
(D_t \bar{u}_{j+\frac{1}{2}}, v_h) + ((\bar{b}\,\nabla\bar{u})_{j+\frac{1}{2}}, \nabla v_h) = (\bar{f}_{j+\frac{1}{2}}, v_h) \quad \forall v_h \in U_h\,.
\tag{5.50}
$$

Hence, subtracting (5.50) from (3.3) gives

$$(\partial_t U_j - D_t \bar{u}_{j+\frac{1}{2}}, v_h) + ((\bar{b}\,\nabla(U-\bar{u}))_{j+\frac{1}{2}}, \nabla v_h) = 0 \quad \forall v_h \in U_h\,. \tag{5.51}$$

Let χ be an arbitrary element in U_h. By adding and subtracting some terms to (5.51) we obtain

$$\begin{aligned}
&(\partial_t(U-\chi)_j, v_h) + ((\bar{b}\,\nabla(U-\chi))_{j+\frac{1}{2}}, \nabla v_h)\\
&= (\partial_t(u-\chi)_j, v_h) + ((\bar{b}\,\nabla(u-\chi))_{j+\frac{1}{2}}, \nabla v_h)\\
&+(D_t\bar{u}_{j+\frac{1}{2}} - \partial_t u_j, v_h) + ((\bar{b}\,\nabla(\bar{u}-u))_{j+\frac{1}{2}}, \nabla v_h) \quad \forall v_h \in U_h.
\end{aligned} \tag{5.52}$$

Now we can choose $v_h = (U-\chi)_{j+\frac{1}{2}}$. From (5.52) and inequalities (2.8) and (5.2) it follows

$$\begin{aligned}
&\frac{1}{2\Delta t}(\|(U-\chi)_{j+1}\|_0^2 - \|(U-\chi)_j\|_0^2) + \lambda_1\|(U-\chi)_{j+\frac{1}{2}}\|_1^2\\
&\leq C\Big(\|\partial_t(u-\chi)_j\|_{-1}^2 + \lambda_2^2\|\nabla(u-\chi)_{j+\frac{1}{2}}\|_0^2 + \|D_t\bar{u}_{j+\frac{1}{2}} - \partial_t u_j\|_{-1}^2\\
&+\lambda_2^2\|\nabla(\bar{u}-u)_{j+\frac{1}{2}}\|_0^2 + \lambda_1\|(U-\chi)_{j+\frac{1}{2}}\|_0^2\Big) + \alpha\|(U-\chi)_{j+\frac{1}{2}}\|_1^2\,,
\end{aligned} \tag{5.53}$$

where we added $\lambda_1\|(U-\chi)_{j+\frac{1}{2}}\|_0^2$ to both sides. Here we used the formula

$$(\partial_t(U-\chi)_j, (U-\chi)_{j+\frac{1}{2}}) = \frac{1}{2\Delta t}(\|(U-\chi)_{j+1}\|_0^2 - \|(U-\chi)_j\|_0^2)\,. \tag{5.54}$$

For (5.53) we need the result (see, e. g., [3], p. 152):

$$\Delta t \sum_{j=0}^{m-1} \|D_t\bar{u}_{j+\frac{1}{2}} - \partial_t u_j\|_{-1}^2 \leq C(\Delta t)^4 \|D_{ttt}u\|_{L^2(\widetilde{H}^{-1})}^2\,. \tag{5.55}$$

Using similar technique it can be proved that

$$\Delta t \sum_{j=0}^{m-1} \|(\bar{u}-u)_{j+\frac{1}{2}}\|_1^2 \leq C(\Delta t)^4\,\|D_{tt}u\|_{L^2(H^1)}^2\,. \tag{5.56}$$

Moreover, it is straight forward to show that

$$\Delta t \sum_{j=0}^{m-1} \|\partial_t(u-\chi)_j\|_{-1}^2 \leq \int_0^{t_m} \|D_t(u-\chi)\|_{-1}^2\,ds \leq \|D_t(u-\chi)\|_{L^2(\widetilde{H}^{-1})}^2\,, \tag{5.57}$$

and

$$\Delta t \sum_{j=0}^{m-1} \|(u-\chi)_{j+\frac{1}{2}}\|_1^2 \leq C\,T\,\|u-\chi\|_{C^0(H^1)}^2\,. \tag{5.58}$$

Finally, by an easy calculation

$$\begin{aligned}&\sum_{j=0}^{m-1} \frac{1}{2\Delta t}\left(\|(U-\chi)_{j+1}\|_0^2 - \|(U-\chi)_j\|_0^2\right)\\ &= \frac{1}{2\Delta t}\left(\|(U-\chi)_{m+1}\|_0^2 - \|U_0-\chi_0\|_0^2\right) .\end{aligned} \tag{5.59}$$

Then, by summing (5.53) for $j = 0, ..., m-1$, choosing $\alpha < \lambda_1$, and using (5.55) - (5.59) we obtain

$$\begin{aligned}&\|(U-\chi)_m\|_0^2 + \Delta t \sum_{j=0}^{m-1} \|(U-\chi)_{j+\frac{1}{2}}\|_1^2\\ &\le C\Delta t \sum_{j=0}^{m-1} (\|\partial_t(u-\chi)_j\|_{-1}^2 + \|\nabla(u-\chi)_{j+\frac{1}{2}}\|_0^2 + \|D_t\bar{u}_{j+\frac{1}{2}} - \partial_t u_j\|_{-1}^2\\ &+\|\nabla(\bar{u}-u)_{j+\frac{1}{2}}\|_0^2 + \|(U-\chi)_{j+\frac{1}{2}}\|_0^2) + \|(U-\chi)_0\|_0^2\\ &\le C\,T\left(\|D_t(u-\chi)\|_{L^2(\widetilde{H}^{-1})}^2 + \|\nabla(u-\chi)\|_{C^0(L^2)}^2 + \|u_{0,h}-u_0\|_0^2\right.\\ &\left.+\|u_0-\chi_0\|_0^2\right) + C(\Delta t)^4(\|D_{ttt}u\|_{L^2(\widetilde{H}^{-1})}^2 + \|D_{tt}u\|_{L^2(H^1)}^2)\\ &+C\Delta t\sum_{j=0}^{m-1}\|(U-\chi)_j\|_0^2\\ &\le C\,T\,h^{2r}(\|D_tu\|_{L^2(H^{r-1})}^2 + \|u\|_{C^0(H^{r+1})}^2 + \|u_0\|_r^2)\\ &+C(\Delta t)^4(\|D_{ttt}u\|_{L^2(\widetilde{H}^{-1})}^2 + \|D_{tt}u\|_{L^2(H^1)}^2) + C\Delta t\sum_{j=0}^{m}\|(U-\chi)_j\|_0^2\\ &\le C\,T\,(h^{2r} + (\Delta t)^4) + C\Delta t\sum_{j=0}^{m}\|(U-\chi)_j\|_0^2 .\end{aligned} \tag{5.60}$$

Here we took χ as the L^2-projection of u and used results from the proof of Lemma 2.1. Using the discrete analogue of Gronwall's inequality, we deduce for Δt sufficiently small

$$\Delta t \sum_{j=0}^{m-1} \|(U-\chi)_{j+\frac{1}{2}}\|_1^2 \le C\,T\,(h^{2r} + (\Delta t)^4) . \tag{5.61}$$

From this it follows, using (5.58) and (5.56)

$$\begin{aligned}&\Delta t\sum_{j=0}^{m-1}\|(U-\bar{u})_{j+\frac{1}{2}}\|_1^2\\ &\le \Delta t\sum_{j=0}^{m-1}\left(\|(U-\chi)_{j+\frac{1}{2}}\|_1^2 + \|(\chi-u)_{j+\frac{1}{2}}\|_1^2 + \|(u-\bar{u})_{j+\frac{1}{2}}\|_1^2\right.\\ &\le C\,T\,(h^{2r} + (\Delta t)^4) .\end{aligned} \tag{5.62}$$

Let $\psi_h \in U_h$ be the L^2-projection of a given $\psi \in \widetilde{H}^1$. Using the equation (5.52), (5.27), and the definition of the $\widetilde{H}^{-1}$-norm we get, like in (5.28)

$$\begin{aligned}
\|\partial_t (U-\chi)_j\|_{-1} &= \sup_{\psi \in \widetilde{H}^1} \frac{(\partial_t (U-\chi)_j, \psi)}{\|\psi\|_1} = \sup_{\psi \in \widetilde{H}^1} \frac{(\partial_t (U-\chi)_j, \psi_h)}{\|\psi\|_1} \\
&\leq C\Big(\|\nabla (U-\chi)_{j+\frac{1}{2}}\|_0 + \|\partial_t (u-\chi)_j\|_{-1} \\
&\quad + \|\nabla (u-\chi)_{j+\frac{1}{2}}\|_0 + \|D_t \bar{u}_{j+\frac{1}{2}} - \partial_t u_j\|_{-1} + \|\nabla (\bar{u}-u)_{j+\frac{1}{2}}\|_0 \Big)
\end{aligned} \tag{5.63}$$

$\forall 0 \leq j \leq m-1$. This together with (5.61), (5.57), (5.58), (5.55), and (5.56) shows

$$\Delta t \sum_{j=0}^{m-1} \|\partial_t U_j - D_t \bar{u}_{j+\frac{1}{2}}\|_{-1}^2 \leq C\,T\,(h^{2r} + (\Delta t)^4)\,, \tag{5.64}$$

which proves the first result.

If we assume that (3.9) is valid, we can show, exactly as in (5.55) that

$$\Delta t \sum_{j=0}^{m-1} \|D_t \bar{u}_{j+\frac{1}{2}} - \partial_t u_j\|_0^2 \leq C(\Delta t)^4 \|D_{ttt} u\|_{L^2(L^2)}^2\,. \tag{5.65}$$

Also, with (3.9) we have, like in (5.56)

$$\Delta t \sum_{j=0}^{m-1} \|(\bar{u}-u)_{j+\frac{1}{2}}\|_2^2 \leq C\,(\Delta t)^4\,\|D_{tt} u\|_{L^2(H^2)}^2\,. \tag{5.66}$$

Moreover, from (5.61) we deduce, using the inverse inequality and the fact $U_h \subset H^2$

$$\begin{aligned}
\Delta t \sum_{j=0}^{m-1} \|(U-\chi)_{j+\frac{1}{2}}\|_2^2 &\leq C\,\Delta t \sum_{j=0}^{m-1} h^{-2}\,\|(U-\chi)_{j+\frac{1}{2}}\|_1^2 \\
&\leq C\,T\,h^{-2}\,(h^{2r} + (\Delta t)^4)\,.
\end{aligned} \tag{5.67}$$

Therefore, as in (5.58) we have

$$\Delta t \sum_{j=0}^{m-1} \|(u-\chi)_{j+\frac{1}{2}}\|_2^2 \leq C\,T\,\|u-\chi\|_{C^0(H^2)}^2 \leq C\,T\,h^{2(r-1)}\,\|u\|_{C^0(H^{r+1})}^2\,. \tag{5.68}$$

A combination of (5.66) - (5.68) proves, as in (5.62)

$$\Delta t \sum_{j=0}^{m-1} \|(U-\bar{u})_{j+\frac{1}{2}}\|_2^2 \leq C\,T\,h^{-2}\,(h^{2r} + (\Delta t)^4)\,. \tag{5.69}$$

Finally, as in (5.63) and (5.29),

$$\begin{aligned}&\|\partial_t(U-\chi)_j\|_0 = \sup_{\psi\in L^2}\frac{(\partial_t(U-\chi)_j,\psi)}{\|\psi\|_0}\\ &\le Ch^{-2}\left(\|\nabla(U-\chi)_{j+\frac12}\|_0+\|\nabla(u-\chi)_{j+\frac12}\|_0+\|\nabla(\bar u-u)_{j+\frac12}\|_0\right)\\ &+\|\partial_t(u-\chi)_j\|_0+\|D_t\bar u_{j+\frac12}-\partial_t u_j\|_0\end{aligned} \tag{5.70}$$

$\forall 0\le j\le m-1$. Hence, the estimate in L^2 between $\partial_t U_j - D_t\bar u_{j+\frac12}$ follows from (5.65) - (5.70) as in (5.64), when using (5.19) and (5.57) for bounding $\|\partial_t(u-\chi)_j\|_0$. This proves the second result.

Proof of Lemma 3.2: As we showed in Lemma 2.2, for h small enough,

$$\begin{aligned}&\lambda_1\le\theta_h\le\lambda_2 \text{ a.e. in } \Omega\,,\\ &\|\nabla\theta_h\|_0\le\mu\,,\\ &\|\theta_h\|_{1,\infty}\le C\end{aligned} \tag{5.71}$$

$\forall t\in[0,T]$, so $\bar\theta_h\in M_h$.

$\widetilde U$ satisfies an equation

$$(\partial_t\widetilde U_j,v_h)+((\bar\theta_h\,\nabla\widetilde U)_{j+\frac12},\nabla v_h)=(\bar f_{j+\frac12},v_h)\quad\forall v_h\in U_h\,. \tag{5.72}$$

Hence, subtracting (3.3) from (5.72) gives

$$\begin{aligned}&(\partial_t(\widetilde U-U)_j,v_h)+((\bar\theta_h\,\nabla(\widetilde U-U))_{j+\frac12},\nabla v_h)\\ &=(((\bar b-\bar\theta_h)\,\nabla U)_{j+\frac12},\nabla v_h)\\ &=(((\bar b-\bar\theta_h)\,\nabla(U-\bar u)_{j+\frac12},\nabla v_h)+(((\bar b-\bar\theta_h)\,\nabla\bar u)_{j+\frac12},\nabla v_h)\\ &\qquad\forall v_h\in U_h\,.\end{aligned} \tag{5.73}$$

As before we choose $v_h=(\widetilde U-U)_{j+\frac12}$. From (5.73) it follows, as in (5.53)

$$\begin{aligned}&\frac{1}{2\Delta t}(\|(\widetilde U-U)_{j+1}\|_0^2-\|(\widetilde U-U)_j\|_0^2)+\lambda_1\|\nabla(\widetilde U-U)_{j+\frac12}\|_0^2\\ &\le C\left(\|\nabla(U-\bar u)_{j+\frac12}\|_0^2+\|(\bar b-\bar\theta_h)_{j+\frac12}\|_0^2\right)+\alpha\|\nabla(\widetilde U-U)_{j+\frac12}\|_0^2\,.\end{aligned} \tag{5.74}$$

Thus, we take again $\alpha<\lambda_1$ and sum (5.74) from 0 to $m-1$ with the additional term $\Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+\frac{1}{2}}\|_0^2$

$$
\begin{aligned}
&\|(\widetilde{U} - U)_m\|_0^2 + \Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+\frac{1}{2}}\|_1^2 \\
&\leq C\Delta t \sum_{j=0}^{m-1} (\|\nabla(U - \bar{u})_{j+\frac{1}{2}}\|_0^2 + \|(\bar{b} - \bar{\theta}_h)_{j+\frac{1}{2}}\|_0^2) \\
&+\Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+\frac{1}{2}}\|_0^2 \\
&\leq C\,T\,(h^{2r} + (\Delta t)^4 + \|b - \theta_h\|_{C^0(L^2)}^2) + \Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+1}\|_0^2 \qquad (5.75) \\
&\leq C\,T\,(h^{2r} + (\Delta t)^4 + h^{2r}\,\|b\|_{C^0(H^r)}^2) + \Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+1}\|_0^2 \\
&\leq C\,T\,(h^{2r} + (\Delta t)^4) + \Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - U)_{j+1}\|_0^2\,,
\end{aligned}
$$

where we used the results from (5.30) and Lemma 3.1. Again, as in Lemma 3.1, it follows from (5.75) that

$$
\Delta t \sum_{j=0}^{m-1} \|(\widetilde{U} - \bar{u})_{j+\frac{1}{2}}\|_1^2 \leq C\,T\,(h^{2r} + (\Delta t)^4)\,. \qquad (5.76)
$$

The estimate in $\widetilde{H}^{-1}$ follows exactly as in (5.63) - (5.64) combined with (5.73). The second estimate of the lemma follows also with the same technique as in (5.65) - (5.70). This ends the proof.

Proof of Lemma 3.3: Because b_h is a minimizer of (3.5), we have, for h small enough, $\Delta t\,J(b_h) \leq \Delta t\,J(\theta_h)$. This means

$$
\begin{aligned}
&\Delta t \sum_{j=0}^{m-1} \Big(\|(W - z_h)_{j+\frac{1}{2}}\|_1^2 + h^2\,(\|\partial_t W_j - \bar{\phi}_{h,j+\frac{1}{2}}\|_0^2 \\
&\qquad + \|\partial_t W_j - \nabla\cdot(\bar{b}_h\,\nabla W)_{j+\frac{1}{2}} - \bar{f}_{h,j+\frac{1}{2}}\|_0^2)\Big) \\
&\leq \Delta t \sum_{j=0}^{m-1} \Big(\|(\widetilde{U} - z_h)_{j+\frac{1}{2}}\|_1^2 + h^2\,(\|\partial_t \widetilde{U}_j - \bar{\phi}_{h,j+\frac{1}{2}}\|_0^2 \qquad (5.77) \\
&\qquad + \|\partial_t \widetilde{U}_j - \nabla\cdot(\bar{\theta}_h\,\nabla \widetilde{U})_{j+\frac{1}{2}} - \bar{f}_{h,j+\frac{1}{2}}\|_0^2)\Big) \\
&= I_1 + I_2 + I_3\,.
\end{aligned}
$$

Using the assumption (2.11), the inverse inequality, and (5.1) we get

$$\begin{aligned}\|u - z_h\|_1 &\le \|u - I_h u\|_1 + C\, h^{-1}\, \|I_h u - z_h\|_0 \\ &\le C\, h^r + C\, h^{-1}\, (\|I_h u - u\|_0 + \|u - z_h\|_0) \\ &\le C\, (h^r + h^{-1}\, \varepsilon_1) \quad \forall t \in [0, T]\,. \end{aligned} \tag{5.78}$$

Thus, using (5.78) and the results of Lemmas 3.1 and 3.2, we proceed with estimates

$$\begin{aligned} I_1 &\le \Delta t \sum_{j=0}^{m-1} 3\, (\|(\widetilde{U} - \bar{u})_{j+\frac{1}{2}}\|_1^2 + \|(\bar{u} - u)_{j+\frac{1}{2}}\|_1^2 + \|(u - z_h)_{j+\frac{1}{2}}\|_1^2) \\ &\le C\, T\, (h^{2r} + (\Delta t)^4 + h^{-2}\, \varepsilon_1^2)\,, \end{aligned} \tag{5.79}$$

$$\begin{aligned} I_2 &\le h^2\, \Delta t \sum_{j=0}^{m-1} 2\, (\|\partial_t \widetilde{U}_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 + \|(D_t \bar{u} - \bar{\phi}_h)_{j+\frac{1}{2}}\|_0^2) \\ &\le C\, T\, (h^{2r} + (\Delta t)^4 + h^2\, \varepsilon_2^2)\,, \end{aligned} \tag{5.80}$$

$$\begin{aligned} I_3 &\le h^2\, \Delta t \sum_{j=0}^{m-1} \Big(\|\partial_t \widetilde{U}_j - \nabla \cdot (\bar{\theta}_h\, \nabla \widetilde{U})_{j+\frac{1}{2}} - \bar{f}_{j+\frac{1}{2}}\|_0^2 + \|(\bar{f} - \bar{f}_h)_{j+\frac{1}{2}}\|_0^2 \Big) \\ &\le C\, h^2 \left(\Delta t \sum_{j=0}^{m-1} \|\partial_t \widetilde{U}_j - \nabla \cdot (\bar{\theta}_h\, \nabla \widetilde{U})_{j+\frac{1}{2}} - D_t \bar{u}_{j+\frac{1}{2}} + \nabla \cdot (\bar{b}\, \nabla \bar{u})_{j+\frac{1}{2}}\|_0^2 \right) \\ &\quad + C\, T\, h^{2r} \\ &\le C\, h^2 \left(\Delta t \sum_{j=0}^{m-1} (\|\partial_t \widetilde{U}_j - D_t \bar{u}_{j+\frac{1}{2}}\|_0^2 + \|(\bar{u} - \widetilde{U})_{j+\frac{1}{2}}\|_2^2 + \right. \\ &\quad \left. \|(\bar{b} - \bar{\theta}_h)_{j+\frac{1}{2}}\|_1^2) \right) \quad + \; C\, T\, h^{2r} \\ &\le C\, T\, (h^{2r} + (\Delta t)^4)\,. \end{aligned} \tag{5.81}$$

Hence, from (5.77) - (5.81) we conclude

$$\begin{aligned} \Delta t \sum_{j=0}^{m-1} & \Big(\|(W - z_h)_{j+\frac{1}{2}}\|_1^2 + h^2\, (\|\partial_t W_j - \bar{\phi}_{h,j+\frac{1}{2}}\|_0^2 \\ & \qquad + \|\partial_t W_j - \nabla \cdot (\bar{b}_h\, \nabla W)_{j+\frac{1}{2}} - \bar{f}_{h,j+\frac{1}{2}}\|_0^2) \Big) \\ & \le C\, T\, (h^{2r} + (\Delta t)^4 + h^{-2}\, \varepsilon_1^2 + h^2\, \varepsilon_2^2)\,. \end{aligned} \tag{5.82}$$

With the previous results we then get

$$\begin{aligned} \Delta t \sum_{j=0}^{m-1} \|(W - \bar{u})_{j+\frac{1}{2}}\|_1^2 &\le \Delta t \sum_{j=0}^{m-1} 2 \Big(\|(W - z_h)_{j+\frac{1}{2}}\|_1^2 + \|(z_h - \bar{u})_{j+\frac{1}{2}}\|_1^2 \Big) \\ &\le C\, T\, (h^{2r} + (\Delta t)^4 + h^{-2}\, \varepsilon_1^2 + h^2\, \varepsilon_2^2)\,, \end{aligned} \tag{5.83}$$

where it follows with the inverse inequality, for $\chi = I_h u$

$$\begin{aligned} \Delta t \sum_{j=0}^{m-1} \|(W-\bar{u})_{j+\frac{1}{2}}\|_2^2 &\le C\,\Delta t \sum_{j=0}^{m-1} \Big(h^{-2}\,\|(W-\bar{\chi})_{j+\frac{1}{2}}\|_1^2 + \|(\bar{\chi}-\bar{u})_{j+\frac{1}{2}}\|_2^2 \\ &\le C\,T\,(h^{2(r-1)} + h^{-2}\,(\Delta t)^4 + h^{-4}\,\varepsilon_1^2 + \varepsilon_2^2)\,, \end{aligned} \tag{5.84}$$

The other two results can be proved similarly starting from (5.82).

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