

A POSTERIORI ERROR ESTIMATES FOR FULLY DISCRETE FRACTIONAL-STEP ϑ -APPROXIMATIONS FOR PARABOLIC EQUATIONS

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ABSTRACT. We derive optimal order a posteriori error estimates for fully discrete approximations of initial and boundary value problems for linear parabolic equations. For the discretisation in time we apply the fractional-step ϑ -scheme and for the discretisation in space the finite element method with finite element spaces that are allowed to change with time. The first optimal order a posteriori error estimates for the norms of $L^\infty(0, T; L^2(\Omega))$ and $L^2(0, T; H^1(\Omega))$ are derived by applying the reconstruction technique.

1. INTRODUCTION

Adaptive finite element methods are a fundamental numerical tool in computational science and engineering for approximating partial differential equations with solutions that exhibit non-trivial characteristics, e.g., [1, 4, 30, 5, 3]. They aim to automatically adjust the mesh to fit the numerical solution, that means fine meshes in the regions where the solution changes fast and coarse in the regions where the solution changes slowly and, consequently, to keep the computational cost as low as possible. The design of such algorithms is usually based on suitable a posteriori error estimates which can measure the quality of the approximate solution and provide information of the error distribution.

In the present paper we derive optimal order a posteriori error estimates for the norms of $L^\infty(0, T; L^2(\Omega))$ and $L^2(0, T; H^1(\Omega))$ for fully discrete fractional-step ϑ -scheme approximations for linear parabolic equations:

$$\begin{cases} u_t - \operatorname{div}(\mathbf{A}\nabla u) = f & \text{in } \Omega \times (0, T], \\ u = 0 & \text{on } \partial\Omega \times (0, T], \\ u(x, 0) = u^0(x) & \text{in } \Omega. \end{cases} \quad (1.1)$$

Here Ω is a convex polyhedral domain in \mathbb{R}^d , $d = 2, 3$, with boundary $\partial\Omega$ and $T > 0$.

We indicate with $\langle \cdot, \cdot \rangle$ the duality pairing in $L^2(\Omega)$ or $H^{-1}(\Omega) - H_0^1(\Omega)$ and we let $a(\cdot, \cdot)$ be defined as $a(u, v) := \langle \mathbf{A}\nabla u, \nabla v \rangle$. For $\mathcal{D} \subset \mathbb{R}^d$ we denote by $\|\cdot\|_{\mathcal{D}}$ the norm in $L^2(\mathcal{D})$, by $\|\cdot\|_{r, \mathcal{D}}$ and by $|\cdot|_{r, \mathcal{D}}$ the norm and the semi-norm, respectively, in the Sobolev space $H^r(\mathcal{D})$, $r \in \mathbb{N}$. In view of the Poincaré inequality, we consider $|\cdot|_{1, \mathcal{D}}$ to be the norm in $H_0^1(\mathcal{D})$ and denote by $|\cdot|_{-1, \mathcal{D}}$ the norm in $H^{-1}(\mathcal{D})$. Whenever $\mathcal{D} = \Omega$ we omit \mathcal{D} in the notation of norms.

We assume throughout that $f \in L^2(0, T; L^2(\Omega))$ and $u^0 \in H_0^1(\Omega)$, and the coefficient matrix $\mathbf{A} = (a_{ij}) \in L^\infty(\Omega)^{d \times d}$ is such that

$$a(v, w) \leq M|v|_1|w|_1 \quad \forall v, w \in H_0^1(\Omega), \quad (1.2)$$

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$$a(v, v) \geq m|v|_1^2 \quad \forall v \in H_0^1(\Omega), \quad (1.3)$$

where M, m are positive constants; then the weak solution u of (1.1) belongs to $L^\infty(0, T; H_0^1(\Omega))$ with $\partial_t u \in L^2(0, T; L^2(\Omega))$.

Although the fractional-step ϑ -scheme was first proposed as an operator splitting method in the context of time-dependent Navier–Stokes equations [15, 16, 11], it is an attractive alternative to popular time-stepping schemes [31, 17]. Indeed, its parameters can be chosen such that to produce a strongly A-stable and second order accurate method. Thus, the scheme can combine the second-order accuracy of the Crank–Nicolson method with the full smoothing property of the backward Euler method in the case of non-smooth initial data. Moreover, in contrast to the backward Euler, it is very little numerically dissipative and, compared to Runge–Kutta methods of higher order, of lower complexity and storage requirements. For more details we refer to [27, 26, 31, 17].

Despite substantial literature on a posteriori error analysis of linear or nonlinear parabolic equations, e.g., [18, 13, 14, 28, 23, 35, 2, 20, 6], the results in case of the fractional-step ϑ -scheme are limited, to our knowledge at least [19, 24, 25]. Particularly, a posteriori error estimates of optimal order in $L^\infty(0, T; L^2(\Omega))$ were derived for time-discrete approximations of linear parabolic equation in [19]. The key for the a posteriori error analysis was the use of a continuous piecewise quadratic in time approximation of u , the so-called *fractional-step ϑ -reconstruction*, whose residual is second order. The definition of the aforementioned reconstruction followed the idea of the *two-point Crank–Nicolson reconstruction* [2].

Here, following the ideas developed in [6, 7], we combine the fractional-step ϑ -scheme and the Galerkin finite element method to get a fully discrete scheme consistent with the mesh modification. The first optimal order a posteriori error estimate in $L^\infty(0, T; L^2(\Omega))$ for fully fractional-step ϑ -approximations are derived by exploiting both the elliptic reconstruction [23], and time-reconstruction techniques [2, 19, 22]. In particular, we define a continuous representation $\widehat{\omega}, \widehat{\omega} : [0, T] \rightarrow H_0^1(\Omega)$, of the approximate solution U , which will be referred to as *space-time reconstruction* of U . The space-time reconstruction $\widehat{\omega}$ is a piecewise quadratic polynomial in time based on approximations on either one time subinterval or two adjacent time subintervals. Then, the *total error* $e := u - U$ may be split as

$$e = u - U = (u - \widehat{\omega}) + (\widehat{\omega} - U) =: \widehat{\rho} + \varepsilon,$$

where

- the *space-time reconstruction error* ε may be split as the sum of the *elliptic reconstruction error* and the *time reconstruction error*. The elliptic reconstruction error can be bounded by using any elliptic estimator at our disposal and the time reconstruction error can be controlled by a posteriori quantities of optimal order.
- the *parabolic error* $\widehat{\rho}$ satisfies an appropriate linear parabolic equation whose right hand-side can be bounded by computable quantities of optimal order.

We note here that the analysis can be extended to more general elliptic spatial operators. Necessary tools in this case are stability estimates for the linear parabolic problem and a posteriori error estimates for the corresponding elliptic problem.

The rest of the paper is organised as follows. In Section 2 we introduce notation and the fully discrete scheme allowing mesh change. In Section 3 we first discuss the space- and time-discretisation and the corresponding reconstructions and then we present the space-time reconstruction. Specific choices of the reconstructions leading to estimators based on approximations on one time subinterval and on two adjacent time subintervals are given. Section 4 is devoted

to the error analysis of the parabolic error $\widehat{\rho}$; we state the final estimates in both aforementioned cases of time-space reconstructions. The asymptotic behaviour of the derived estimators is studied in Section 5.

2. PRELIMINARIES

In this section we introduce the necessary notation for our analysis and the fully discrete scheme.

2.1. Notation. Let $0 = t^0 < t^1 < \dots < t^N = T$, $I_n := (t^{n-1}, t^n]$ and $k_n := t^n - t^{n-1}$. For $\vartheta \in (0, \frac{1}{3})$, we introduce the intermediate time levels $t^{n-1+\vartheta} = t^{n-1} + \vartheta k_n$ and $t^{n-\vartheta} = t^{n-1} + (1-\vartheta)k_n$.

For each $0 \leq n \leq N$, let \mathcal{T}_n be a triangulation of Ω into disjoint d -simplices K and h_n its *local mesh-size function* defined by

$$h_n(x) := \text{diam}(K), \quad K \in \mathcal{T}_n \text{ and } x \in K. \quad (2.1)$$

We assume that the aspect ratios of all the elements are uniformly bounded with respect to $n = 0, \dots, N$, and the intersection of two different elements is either empty, or consists of a common vertex, a common edge, or a common face.

We associate with each \mathcal{T}_n the following two finite element spaces

$$\widetilde{\mathbb{V}}^n := \{\phi \in H^1(\Omega) : \forall K \in \mathcal{T}_n : \phi|_K \in \mathbb{P}^l(K)\} \quad \text{and} \quad \mathbb{V}^n := \widetilde{\mathbb{V}}^n \cap H_0^1(\Omega), \quad (2.2)$$

where, for $l \geq 0$, $\mathbb{P}^l(D)$ is the space of polynomials of degree at most l on D .

For a simplex K , we denote by $\mathcal{E}(K)$ the set of sides of K (edges in $d = 2$ or faces in $d = 3$) and by $\Sigma(K) \subset \mathcal{E}(K)$ the set of the internal sides of K , namely sides that are contained in the interior of Ω . In addition, we introduce the sets $\mathcal{E}_n := \cup_{K \in \mathcal{T}_n} \mathcal{E}(K)$ and $\Sigma_n := \cup_{K \in \mathcal{T}_n} \Sigma(K)$.

Let us now make assumptions on the family of triangulations $(\mathcal{T}_n)_{n \in \{0, 1, \dots, N\}}$ that allow us to derive the a posteriori error estimates. We refer to Appendices A and B in [20] for more details. Let \mathcal{M} be a shape-regular macro-triangulation of Ω . We assume that each triangulation \mathcal{T}_n , $n = 1, \dots, N$, is derived from \mathcal{M} by using an admissible refinement procedure, e.g., the bisection-based refinement procedure used in ALBERTA-FEM toolbox [32]. Under this assumption the shape-regularity of the mesh is preserved. Moreover, given two refinements \mathcal{T} and \mathcal{T}' of \mathcal{M} , this assumption assures that for any elements $K \in \mathcal{T}$ and $K' \in \mathcal{T}'$, either $K \cap K' = \emptyset$, $K \subset K'$ or $K' \subset K$.

A set of refinements of \mathcal{M} can be enriched with a partial order relation: we write $\mathcal{T} \leq \mathcal{T}'$ if \mathcal{T}' is a refinement of \mathcal{T} . Given two successive triangulations \mathcal{T}_{n-1} and \mathcal{T}_n , we denote by $\widehat{\mathcal{T}}_n$ their *finest common coarsening*, that is the finest triangulation satisfying $\widehat{\mathcal{T}}_n \leq \mathcal{T}_{n-1}$ and $\widehat{\mathcal{T}}_n \leq \mathcal{T}_n$. Similarly, we introduce the *coarsest common refinement* $\check{\mathcal{T}}_n$ to be the coarsest triangulation that satisfies $\mathcal{T}_{n-1} \leq \check{\mathcal{T}}_n$ and $\mathcal{T}_n \leq \check{\mathcal{T}}_n$. Then, $\widehat{h}_n := \max(h_n, h_{n-1})$ and $\check{h}_n := \min(h_n, h_{n-1})$, respectively.

In addition, we shall denote by $\check{\Sigma}_n$ and $\widehat{\Sigma}_n$ the sets of the interior sides corresponding to $\check{\mathcal{T}}_n$ and $\widehat{\mathcal{T}}_n$, respectively, namely $\check{\Sigma}_n := \cup_{K \in \check{\mathcal{T}}_n} \Sigma(K)$ and $\widehat{\Sigma}_n := \cup_{K \in \widehat{\mathcal{T}}_n} \Sigma(K)$.

We shall use the shorthand notation $u^m(\cdot) := u(\cdot, t^m)$ and $f^m(\cdot) := f(\cdot, t^m)$ throughout. The jump $J[\mathbf{v}]_e$ of a vector valued function \mathbf{v} across an interior side $e \in \Sigma(K)$ is defined by

$$J[\mathbf{v}]_e(x) := \lim_{\delta \rightarrow 0} [\mathbf{v}(x + \delta \mathbf{n}_e) - \mathbf{v}(x - \delta \mathbf{n}_e)] \cdot \mathbf{n}_e, \quad (2.3)$$

where $x \in e$ and \mathbf{n}_e denotes a unit normal vector to e with fixed but arbitrary orientation. We shall omit the subindex e when it is clear from the context.

In addition, we shall use the following notation for functions v defined in a piecewise sense

$$\begin{aligned} \|h_n^i v\|_{\mathcal{T}_n} &= \left(\sum_{K \in \mathcal{T}_n} \|h_K^i v\|_K^2 \right)^{1/2}, \\ \|h_n^{i+\frac{1}{2}} J[\nabla v]\|_{\Sigma_n} &= \left(\sum_{e \in \Sigma_n} \|h_e^{i+\frac{1}{2}} J[\nabla v]_e\|_e^2 \right)^{1/2}, \end{aligned} \quad i = 1, 2. \quad (2.4)$$

2.2. Discrete and interpolation operators. For $0 \leq n \leq N$, let $A^n : H_0^1(\Omega) \rightarrow \mathbb{V}^n$ be the discrete elliptic operator corresponding to the finite element space \mathbb{V}^n defined by

$$\langle A^n v, \chi_n \rangle = a(v, \chi_n) \quad \forall \chi_n \in \mathbb{V}^n. \quad (2.5)$$

Moreover, we denote by $P_0^n : L^2(\Omega) \rightarrow \mathbb{V}^n$ the L^2 -projection and by $\Pi^n, \tilde{\Pi}^n : \mathbb{V}^{n-1} \rightarrow \mathbb{V}^n$ projection or interpolation operators to be appropriately chosen. The choice of projection or interpolation operators passing information from the previous finite element space to the one corresponding to the next time step might be crucial for an adaptive algorithm [8, 7, 9, 10] and nonstandard projections with improved smoothing properties might be desirable. We emphasise here that our analysis does not require any specific assumptions on the choice of $\Pi^n, \tilde{\Pi}^n$ and the use of nonstandard projections is also allowed.

For the purpose of the proofs of the a posteriori error estimates we let $\mathcal{I}^n : H_0^1(\Omega) \rightarrow \mathbb{V}^n$ be a Clément-type interpolation operator. For completeness, we recall the definition of Clément interpolation operator introduced in [12] as well as its stability and its approximation properties. The interpolation operator of Scott and Zhang [33] could also have been used, particularly in the case of non-homogeneous boundary conditions.

Definition 2.1 (Clément interpolation operator). *Let \mathcal{N}_n be the set of internal vertices of \mathcal{T}_n . Let $\omega_i := \text{supp}(\varphi_i)$ be the support of a piecewise linear basis function φ_i associated with the vertex $p_i \in \mathcal{N}_n$. Then, the Clément interpolation operator $\mathcal{I}^n : H_0^1(\Omega) \rightarrow \mathbb{V}^n$ is defined by*

$$\mathcal{I}^n v(x) = \sum_{p_i \in \mathcal{N}_n} v_i(p_i) \varphi_i(x), \quad (2.6)$$

where v_i is the local $L^2(\omega_i)$ -projection of $v \in H_0^1(\Omega)$ given by

$$\langle v - v_i, q \rangle_{L^2(\omega_i)} = 0 \quad \forall q \in \mathbb{P}_1(\omega_i). \quad (2.7)$$

Lemma 2.2 (Stability and interpolation properties). *Let $\mathcal{I}^n : H_0^1(\Omega) \rightarrow \mathbb{V}^n$ be a Clément interpolation operator. Then, we have the H^1 -stability of \mathcal{I}^n ,*

$$|\mathcal{I}^n z|_1 \leq c_1 |z|_1. \quad (2.8)$$

Furthermore, for $j \leq l + 1$, the following approximation properties are satisfied

$$\begin{aligned} \|h_n^{-j} (z - \mathcal{I}^n z)\|_{\mathcal{T}_n} &\leq c_{1,j} |z|_j, \\ \|h_n^{1/2-j} (z - \mathcal{I}^n z)\|_{\Sigma_n} &\leq c_{2,j} |z|_j, \end{aligned} \quad (2.9)$$

where l is the finite element polynomial degree and the constants $c_1, c_{1,j}$ and $c_{2,j}$ depend only on the shape-regularity of the family of triangulations $\{\mathcal{T}_n\}_{n=0}^N$.

Let C_E denote the elliptic regularity constant, that is

$$\|v\|_2 \leq C_E \|\text{div}(\mathbf{A}\nabla v)\|, \quad v \in H^2(\Omega) \cap H_0^1(\Omega), \quad (2.10)$$

and $c_1, c_{i,j}, i = 1, 2, j \leq l + 1$, be the constants in Lemma 2.2.

We shall also use the notation

$$C_{j,2} := C_E c_{j,2}$$

for the constants appearing in the definition of the a posteriori error estimators.

2.3. The fully discrete scheme. We discretise (1.1) by applying the following Galerkin fractional-step ϑ -scheme (GFS-scheme): for a given approximation U^0 of u^0 and for $1 \leq n \leq N$, assuming that U^{n-1} has been computed, find $U^n \in \mathbb{V}^n$, and the intermediate $U^{n-1+\vartheta}, U^{n-\vartheta}$, such that

$$\left\{ \begin{array}{l} \frac{U^{n-1+\vartheta} - \Pi^n U^{n-1}}{\vartheta k_n} + \alpha_1 A^n U^{n-1+\vartheta} + \beta_1 \tilde{\Pi}^n A^{n-1} U^{n-1} = P_0^n (\alpha_2 f^{n-1+\vartheta} + \beta_2 f^{n-1}), \\ \frac{U^{n-\vartheta} - U^{n-1+\vartheta}}{(1-2\vartheta)k_n} + \beta_1 A^n U^{n-\vartheta} + \alpha_1 A^n U^{n-1+\vartheta} = P_0^n (\beta_2 f^{n-\vartheta} + \alpha_2 f^{n-1+\vartheta}), \\ \frac{U^n - U^{n-\vartheta}}{\vartheta k_n} + \alpha_1 A^n U^n + \beta_1 A^n U^{n-\vartheta} = P_0^n (\alpha_2 f^n + \beta_2 f^{n-\vartheta}), \end{array} \right. \quad (2.11)$$

with $\alpha_1, \alpha_2 \in (0, 1)$, and $\beta_1 = 1 - \alpha_1, \beta_2 = 1 - \alpha_2$. We shall sometimes find it convenient to rewrite (2.11) in the form

$$\left\{ \begin{array}{l} \frac{U^{n-1+\vartheta} - \Pi^n U^{n-1}}{k_n} + \alpha_1 \vartheta A^n U^{n-1+\vartheta} + \beta_1 \vartheta \tilde{\Pi}^n A^{n-1} U^{n-1} \\ = P_0^n (\alpha_2 \vartheta f^{n-1+\vartheta} + \beta_2 \vartheta f^{n-1}), \\ \frac{U^{n-\vartheta} - \Pi^n U^{n-1}}{k_n} + \beta_1 (1-2\vartheta) A^n U^{n-\vartheta} + \alpha_1 (1-\vartheta) A^n U^{n-1+\vartheta} + \beta_1 \vartheta \tilde{\Pi}^n A^{n-1} U^{n-1} \\ = P_0^n (\beta_2 (1-2\vartheta) f^{n-\vartheta} + \alpha_2 (1-\vartheta) f^{n-1+\vartheta} + \beta_2 \vartheta f^{n-1}), \\ \frac{U^n - \Pi^n U^{n-1}}{k_n} + \alpha_1 \vartheta A^n U^n + \beta_1 (1-\vartheta) A^n U^{n-\vartheta} + \alpha_1 (1-\vartheta) A^n U^{n-1+\vartheta} \\ + \beta_1 \vartheta \tilde{\Pi}^n A^{n-1} U^{n-1} \\ = P_0^n (\alpha_2 \vartheta f^n + \beta_2 (1-\vartheta) f^{n-\vartheta} + \alpha_2 (1-\vartheta) f^{n-1+\vartheta} + \beta_2 \vartheta f^{n-1}). \end{array} \right. \quad (2.12)$$

Throughout the rest of the paper we shall assume that $\vartheta = 1 - \frac{\sqrt{2}}{2}$ and $\alpha_1 \in (\frac{1}{2}, 1]$, which implies that the fractional-step ϑ -scheme is second-order accurate and $A(0)$ -stable. Indeed, the assumption that $\alpha_1 \in (\frac{1}{2}, 1]$ implies the strong A -stability of our scheme. Furthermore, we can easily see that the quadrature rule

$$\mathcal{I}_{\alpha, \vartheta}(\phi) := \beta \vartheta \phi(0) + \alpha (1 - \vartheta) \phi(\vartheta) + \beta (1 - \vartheta) \phi(1 - \vartheta) + \alpha \vartheta \phi(1) \approx \int_0^1 \phi(s) ds \quad (2.13)$$

is exact for polynomials of degree at most one if and only if $\alpha = \beta = \frac{1}{2}$ or $\vartheta = 1 - \frac{\sqrt{2}}{2}$. Thus, the assumption $\vartheta = 1 - \frac{\sqrt{2}}{2}$ ensures that the fractional-step ϑ -scheme is second-order accurate with respect to time. We refer to [17] for more details.

2.4. The fully discrete scheme in compact form. We introduce the following piecewise linear polynomials with respect to time

$$\varphi(t) := \ell_0^n(t) f^{n-1} + \ell_1^n(t) f^n, \quad t \in I_n, \quad (2.14)$$

and

$$\Theta(t) = \ell_0^n(t) \tilde{\Pi}^n A^{n-1} U^{n-1} + \ell_1^n(t) A^n U^n, \quad t \in I_n, \quad (2.15)$$

with

$$\ell_0^n(t) := \frac{t^n - t}{k_n} \quad \text{and} \quad \ell_1^n(t) := \frac{t - t^{n-1}}{k_n}, \quad t \in I_n. \quad (2.16)$$

Moreover, we let $\widehat{\Theta}$ be defined as

$$\widehat{\Theta}(t) := \Theta(t) - \xi_{\Theta}^n, \quad t \in I_n, \quad (2.17)$$

with

$$\xi_{\Theta}^n := (1 - \vartheta) \left(\alpha \left[\Theta(t^{n-1+\vartheta}) + A^n U^{n-1+\vartheta} \right] + \beta \left[\Theta(t^{n-\vartheta}) + A^n U^{n-\vartheta} \right] \right), \quad t \in I_n, \quad (2.18)$$

and $\widehat{\varphi}$

$$\widehat{\varphi}(t) := \varphi(t) - \xi_{\varphi}^n, \quad t \in I_n, \quad (2.19)$$

with

$$\xi_{\varphi}^n := (1 - \vartheta) \left(\alpha \left[\varphi(t^{n-1+\vartheta}) - f^{n-1+\vartheta} \right] + \beta \left[\varphi(t^{n-\vartheta}) - f^{n-\vartheta} \right] \right), \quad t \in I_n. \quad (2.20)$$

Note that both ξ_{Θ}^n and ξ_{φ}^n are a posteriori quantities of optimal order, cf. [19] for details.

According to definitions (2.17) and (2.19) the last substep of the fractional-step ϑ -scheme may be written in the following compact form

$$\frac{U^n - \Pi^n U^{n-1}}{k_n} + \widehat{\Theta}(t^{n-\frac{1}{2}}) = P_0^n \widehat{\varphi}(t^{n-\frac{1}{2}}). \quad (2.21)$$

3. SPACE-TIME RECONSTRUCTIONS

As aforementioned, the a posteriori error estimates will be derived by using the reconstruction technique. Our goal is to define a continuous representation $\widehat{\omega}$ of the approximate solution, $\widehat{\omega} : [0, T] \rightarrow H_0^1(\Omega)$, which will be a second order approximation of the exact solution $u(t)$ and whose residual will also be second order accurate. To define $\widehat{\omega}(t)$ we shall exploit both the ideas of *elliptic reconstruction* introduced in [23] and the fractional-step ϑ -reconstruction based on approximations on one time subinterval introduced in [19]. Additionally, we shall extend the idea of the three-point Crank–Nicolson reconstruction [22, 29] and shall define a second fractional-step ϑ -reconstruction which will be based on approximations on two adjacent time subintervals. We shall begin our discussion by recalling the definition of the elliptic reconstruction operator and its basic properties.

3.1. Reconstruction in space. To derive a posteriori error estimates of optimal order in the $L^\infty(0, T; L^2(\Omega))$ -norm for finite element discretisations of parabolic equations, the use of the elliptic reconstruction is necessary. The elliptic reconstruction may be regarded as an a posteriori analogue to the elliptic projection appearing in standard a priori error analysis for parabolic problems [36, 34]. Note that in the fully discrete case, with the finite element spaces allowed to change with time, the elliptic reconstruction operator depends on n .

Definition 3.1 (Elliptic reconstruction). *For fixed $v_n \in \mathbb{V}^n$, we define the elliptic reconstruction $\mathcal{R}^n v_n \in H_0^1(\Omega)$ of v_n , as the solution of the following elliptic problem*

$$a(\mathcal{R}^n v_n, \psi) = \langle A^n v_n, \psi \rangle \quad \forall \psi \in H_0^1(\Omega). \quad (3.1)$$

It can be easily seen that the elliptic reconstruction \mathcal{R}^n satisfies the Galerkin orthogonality property

$$a(\mathcal{R}^n v_n - v_n, \chi_n) = 0 \quad \forall \chi_n \in \mathbb{V}^n. \quad (3.2)$$

For completeness we shall next give residual-based a posteriori estimates for the elliptic reconstruction error $(\mathcal{R}^n - I)v_n$.

Lemma 3.2 (Residual-based a posteriori estimates for the elliptic reconstruction error). *Let $v_n \in \mathbb{V}^n$ and $\mathcal{R}^n v_n$ be its elliptic reconstruction defined as in (3.1). Then, the following estimates hold true*

$$|(\mathcal{R}^n - I)v_n|_1 \leq \eta_{1,n}(v_n), \quad (3.3)$$

$$\|(\mathcal{R}^n - I)v_n\| \leq \eta_{2,n}(v_n), \quad (3.4)$$

where $\eta_{1,n}$ and $\eta_{2,n}$ are the elliptic estimators given by

$$\eta_{1,n}(v_n) := \frac{c_{1,1}}{m} \|h_n(\operatorname{div}(\mathbf{A}\nabla) + A^n)v_n\|_{\mathcal{T}_n} + \frac{c_{2,1}}{m} \|h_n^{1/2} J[\mathbf{A}\nabla v_n]\|_{\Sigma_n}, \quad (3.5)$$

$$\eta_{2,n}(v_n) := C_{1,2} \|h_n^2(\operatorname{div}(\mathbf{A}\nabla) + A^n)v_n\|_{\mathcal{T}_n} + C_{2,2} \|h_n^{3/2} J[\mathbf{A}\nabla v_n]\|_{\Sigma_n}. \quad (3.6)$$

We shall now turn our discussion to the time discretisation and the so-called fractional-step ϑ -reconstruction.

3.2. Reconstruction in time. Regarding the temporal variable, our goal is to define a second order approximation $U(t)$ of $u(t)$, for all $t \in [0, T]$, whose residual is also second order accurate. Choosing $U : [0, T] \rightarrow H_0^1(\Omega)$ to be the piecewise linear interpolant at the nodal values, that is

$$U(t) := \ell_0^n(t) U^{n-1} + \ell_1^n(t) U^n, \quad t \in I_n, \quad (3.7)$$

where ℓ_0^n and ℓ_1^n are defined in (2.16), may seem natural for a second-order accurate scheme. Indeed, since the error at the nodes is of second order, $U(t)$ is an approximation of $u(t)$ of the same order, for all $t \in [0, T]$. However, its residual $R_U(t)$

$$R_U(t) := U_t(t) - \operatorname{div}(\mathbf{A}\nabla U)(t) - f(t), \quad t \in I_n, \quad (3.8)$$

is an a posteriori quantity of first order with respect to time. We observe, using (1.1), that $R_U(t)$ may be written also in the form

$$R_U(t) = [U_t(t) - u_t(t)] - \operatorname{div}(\mathbf{A}(\nabla U - \nabla u))(t), \quad t \in I_n. \quad (3.9)$$

Although the second term on the right-hand side is of second order with respect to time, we note that the first term is of first order only.

By applying energy techniques to this error equation we can only derive residual-based a posteriori error estimates of suboptimal order with respect to time.

To recover the second order of accuracy in time, we shall define appropriate reconstructions \widehat{U} in time which will be piecewise quadratic polynomials based on approximations on one time subinterval as well as on approximations based on two time subintervals.

Definition 3.3 (Time reconstructions). *We introduce the piecewise quadratic time reconstruction $\widehat{U} : [0, T] \rightarrow H_0^1(\Omega)$, as follows*

$$\widehat{U}(t) := U(t) + \frac{1}{2}(t - t^{n-1})(t - t^n)w_n, \quad t \in I_n, \quad (3.10)$$

$n = 1, \dots, N$, where w_n is an appropriate element of $H_0^1(\Omega)$.

In view of (3.3) and by observing that

$$\int_{t^{n-1}}^{t^n} (t - t^{n-1})^2 (t^n - t)^2 dt = \frac{k_n^5}{30}, \quad (3.11)$$

we can easily see that the following result holds true.

Lemma 3.4 (Time reconstruction error estimates). *For $n = 1, \dots, N$, the following estimates hold true*

$$\left(\int_{t^{n-1}}^{t^n} |(\widehat{U} - U)(t)|_1^2 \right)^{1/2} \leq \frac{k_n^{5/2}}{2\sqrt{30}} |w_n|_1, \quad (3.12)$$

$$\max_{t^{n-1} \leq t \leq t^n} \|(\widehat{U} - U)(t)\| \leq \frac{k_n^2}{8} \|w_n\|. \quad (3.13)$$

In the sequel we shall study two choices for the time reconstruction \widehat{U} which correspond to two appropriate choices for w_n . In particular, we shall consider the following cases:

Time reconstruction 1 (based on approximations on one time subinterval): We shall extend the idea of the fractional-step ϑ -reconstruction introduced in [19] to the fully discrete case. For this purpose we choose w_n in (3.10) as

$$w_n := \Theta_t(t) - P_0^n \varphi_t(t) = \frac{A^n U^n - \widetilde{\Pi}^n A^{n-1} U^{n-1}}{k_n} - \frac{P_0^n (f^n - f^{n-1})}{k_n}, \quad t \in I_n. \quad (3.14)$$

Time reconstruction 2 (based on approximations on two adjacent time subintervals): The so-called three-point quadratic reconstruction for the Crank–Nicolson scheme [22, 29] is defined by choosing w_n to be a finite difference approximation of u_{tt} that uses the approximations on two adjacent time subintervals. Based on this idea, we define a three time-level quadratic reconstruction for the GFS-scheme by replacing w_n in (3.10) with

$$\widetilde{w}_n := -\frac{2}{k_n + k_{n-1}} \left(\left[\frac{U^n - \Pi^n U^{n-1}}{k_n} \right] - \pi^n \left[\frac{U^{n-1} - \Pi^{n-1} U^{n-2}}{k_{n-1}} \right] \right), \quad (3.15)$$

where π^n is any projection to \mathbb{V}^n at our disposal.

3.3. Reconstruction in space and time. The construction of appropriate space-time reconstructions for our analysis combines the ideas discussed in the previous two paragraphs. Let $\omega : [0, T] \rightarrow H_0^1(\Omega)$ be the piecewise linear in time function defined by linearly interpolating between the values $\mathcal{R}^{n-1} U^{n-1}$ and $\mathcal{R}^n U^n$,

$$\omega(t) := \ell_0^n(t) \mathcal{R}^{n-1} U^{n-1} + \ell_1^n(t) \mathcal{R}^n U^n, \quad t \in I_n, \quad (3.16)$$

with ℓ_0^n and ℓ_1^n as in (2.16). According to the discussion above, the use of ω as intermediate function will lead to sub-optimal error estimates. The introduction of a piecewise quadratic polynomial in time is necessary, therefore we define the space-time reconstruction $\widehat{\omega}$ of the approximate solution U :

Definition 3.5 (Space–time reconstruction). *We introduce the space-time reconstruction $\widehat{\omega} : [0, T] \rightarrow H_0^1(\Omega)$ of the approximate solution U as follows*

$$\widehat{\omega}(t) := \omega(t) + \frac{1}{2}(t - t^{n-1})(t^n - t) \mathcal{R}^n w_n. \quad (3.17)$$

We shall now derive $L^2(0, T; H^1(\Omega))$ and $L^\infty(0, T; L^2(\Omega))$ estimates for the space-time reconstruction error $\varepsilon = \widehat{\omega} - U$. The error ε may be written as the sum of the *elliptic reconstruction error* ϵ and the *time reconstruction error* σ , that is

$$\widehat{\omega} - U = \epsilon + \sigma, \quad \text{where } \epsilon := \omega - U, \quad \sigma := \widehat{\omega} - \omega. \quad (3.18)$$

According to (3.4) and (3.13) the following upper bounds for the reconstruction errors ϵ and σ are valid.

Lemma 3.6 ($L^2(H^1)$ error estimates for the reconstruction error). *For $m = 1, \dots, N$, the following estimate holds true*

$$\left(\int_0^{t^m} |\epsilon(t)|_1^2 \right)^{1/2} \leq \mathcal{E}_{1,m}^{\text{ell}} \quad \text{with} \quad \mathcal{E}_{1,m}^{\text{ell}} := \left(\sum_{n=1}^m k_n (\eta_{1,n-1}^2(U^{n-1}) + \eta_{1,n}^2(U^n)) \right)^{1/2}, \quad (3.19)$$

where $\eta_{1,n}$ is defined in (3.5). Furthermore,

$$\left(\int_0^{t^m} |\sigma(t)|_1^2 \right)^{1/2} \leq \mathcal{E}_{1,m}^{\text{rec}}(w_n), \quad (3.20)$$

where

$$\mathcal{E}_{1,m}^{\text{rec}}(w_n) := \left(\sum_{n=1}^m k_n \gamma_n^2(w_n) \right)^{1/2} \quad \text{with} \quad \gamma_n(w_n) := \frac{k_n^2}{2\sqrt{30}} (c_1 M |w_n|_1 + C_{1,1} \|h_n A^n w_n\|). \quad (3.21)$$

Proof. First, the estimate (3.19) can be easily derived. Next, we show the estimate (3.20). We have

$$|\sigma(t)|_1^2 = a(\sigma(t), \sigma(t)) = \frac{1}{2} (t - t^{n-1})(t^n - t) a(\mathcal{R}^n w_n, \sigma(t)). \quad (3.22)$$

By using the definition of the elliptic reconstruction (3.1), we get

$$|\sigma(t)|_1 \leq \frac{1}{2} (t - t^{n-1})(t^n - t) |A^n w_n|_{-1}.$$

To estimate the dual norm in the above relation, we can proceed as follows

$$\begin{aligned} |A^n w_n|_{-1} &= \sup_{0 \neq z \in H_0^1(\Omega)} \frac{\langle A^n w_n, z \rangle}{|z|_1} \\ &= \sup_{0 \neq z \in H_0^1(\Omega)} \left\{ \frac{\langle A^n w_n, \mathcal{I}^n z \rangle}{|z|_1} + \frac{\langle A^n w_n, z - \mathcal{I}^n z \rangle}{|z|_1} \right\}, \end{aligned} \quad (3.23)$$

with $\mathcal{I}^n z \in \mathbb{V}^n$ a Clément-type interpolant of z . Now, in view of (2.5), (1.2) and (2.8), we have

$$\langle A^n w_n, \mathcal{I}^n z \rangle \leq c_1 M |w_n|_1 |z|_1. \quad (3.24)$$

Furthermore, using the approximation properties (2.9) of a Clément-type interpolation operator, we obtain

$$\langle A^n w_n, z - \mathcal{I}^n z \rangle \leq c_{1,1} \|h_n A^n w_n\| |z|_1. \quad (3.25)$$

According to (3.24) and (3.25), (3.23) leads to

$$|A^n w_n|_{-1} \leq c_1 M |w_n|_1 + C_{1,1} \|h_n A^n w_n\|. \quad (3.26)$$

By using again (3.11) the claimed result follows. \square

Lemma 3.7 ($L^\infty(L^2)$ error estimates for the reconstruction error). *For $m = 1, \dots, N$, the following estimates hold*

$$\max_{0 \leq t \leq t^m} \|\epsilon(t)\| \leq \mathcal{E}_{2,m}^{\text{ell}} \quad \text{with} \quad \mathcal{E}_{2,m}^{\text{ell}} := \max_{0 \leq n \leq m} \eta_{2,n}(U^n) \quad (3.27)$$

and

$$\max_{0 \leq t \leq t^m} \|\sigma(t)\| \leq \mathcal{E}_{2,m}^{\text{rec}}(w_n) \quad \text{with} \quad \mathcal{E}_{2,m}^{\text{rec}}(w_n) := \max_{0 \leq n \leq m} \frac{k_n^2}{8} \{ \eta_{2,n}(w_n) + \|w_n\| \}, \quad (3.28)$$

where $\eta_{2,n}$ is defined in (3.6).

4. $L^2(H^1)$ AND $L^\infty(L^2)$ ESTIMATES FOR THE TOTAL ERROR

Let ρ , $\widehat{\rho}$ denote the *parabolic errors* defined by $\rho := u - \omega$, $\widehat{\rho} := u - \widehat{\omega}$, respectively. The *total error* $e := u - U$ can be split as follows

$$e = u - U = (u - \widehat{\omega}) + (\widehat{\omega} - U) = \widehat{\rho} + \sigma + \epsilon. \quad (4.1)$$

A bound for the reconstruction error $\sigma + \epsilon$ was presented in the previous section. We shall now continue with the estimation of the basic parabolic error, which is stated in Theorem 4.2.

4.1. An a posteriori estimate in $L^\infty(L^2)$ and $L^2(H^1)$ for the parabolic error. We begin with the derivation of the error equation:

Lemma 4.1 (Error equation). *For each $t \in I_n$, it holds*

$$\langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) = \langle R_n(t), \psi \rangle \quad \forall \psi \in H_0^1(\Omega), \quad (4.2)$$

with

$$\begin{aligned} R_n(t) := & \ell_0^n(t)(\Pi^n - I)A^{n-1}U^{n-1} - k_n^{-1}(\Pi^n - I)U^{n-1} - (t - t^{n-\frac{1}{2}})(\mathcal{R}^n - I)w_n \\ & - (t - t^{n-\frac{1}{2}})(w_n - \Theta_t(t) + P_0^n \varphi_t(t)) - \frac{(\mathcal{R}^{n-1} - I)U^{n-1} - (\mathcal{R}^n - I)U^n}{k_n} \\ & + \xi_{\Theta}^n + f(t) - P_0^n \widehat{\varphi}(t). \end{aligned} \quad (4.3)$$

Proof. For $n = 1, \dots, N$, and $\psi \in H_0^1$, in view of (3.16) and (3.17), we obtain

$$\langle \widehat{\omega}_t(t), \psi \rangle = \langle \omega_t(t), \psi \rangle + (t - t^{n-\frac{1}{2}})\langle \mathcal{R}^n w_n, \psi \rangle. \quad (4.4)$$

Thus, by using Definition 3.5, we get

$$\begin{aligned} \langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) = & -a(\ell_0^n(t)\mathcal{R}^{n-1}U^{n-1} + \ell_1^n(t)\mathcal{R}^n U^n, \psi) - (t - t^{n-\frac{1}{2}})\langle \mathcal{R}^n w_n, \psi \rangle \\ & - k_n^{-1}\langle \mathcal{R}^n U^n - \mathcal{R}^{n-1}U^{n-1}, \psi \rangle + \langle f(t), \psi \rangle. \end{aligned}$$

According to the elliptic reconstruction definition (3.1), the last relation leads to

$$\begin{aligned} \langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) = & -\langle \ell_0^n(t)(A^{n-1}U^{n-1} + \ell_1^n(t)A^n U^n, \psi) \\ & - (t - t^{n-\frac{1}{2}})\langle \mathcal{R}^n w_n, \psi \rangle - k_n^{-1}\langle \mathcal{R}^n U^n - \mathcal{R}^{n-1}U^{n-1}, \psi \rangle + \langle f(t), \psi \rangle, \end{aligned} \quad (4.5)$$

from which, in view of (2.15), we infer that

$$\begin{aligned} \langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) = & -\langle \Theta(t), \psi \rangle + \ell_0^n(t)\langle (\Pi^n - I)A^{n-1}U^{n-1}, \psi \rangle \\ & - (t - t^{n-\frac{1}{2}})\langle (\mathcal{R}^n - I)w_n, \psi \rangle - (t - t^{n-\frac{1}{2}})\langle w_n, \psi \rangle \\ & - k_n^{-1}\langle (\mathcal{R}^{n-1} - I)U^{n-1} - (\mathcal{R}^n - I)U^n, \psi \rangle \\ & + k_n^{-1}\langle U^n - U^{n-1}, \psi \rangle + \langle f(t), \psi \rangle. \end{aligned} \quad (4.6)$$

Now, in view of (2.21), we observe that

$$\begin{aligned} \langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) = & \ell_0^n(t)\langle (\Pi^n - I)A^{n-1}U^{n-1} - k_n^{-1}(\Pi^n - I)U^{n-1}, \psi \rangle \\ & - (t - t^{n-\frac{1}{2}})\langle (\mathcal{R}^n - I)w_n, \psi \rangle - (t - t^{n-\frac{1}{2}})\langle w_n, \psi \rangle + \langle \widehat{\Theta}(t^{n-\frac{1}{2}}) - P_0^n \widehat{\varphi}(t^{n-\frac{1}{2}}), \psi \rangle \\ & - k_n^{-1}\langle (\mathcal{R}^{n-1} - I)U^{n-1} - (\mathcal{R}^n - I)U^n, \psi \rangle - \langle \Theta(t), \psi \rangle + \langle f(t), \psi \rangle. \end{aligned} \quad (4.7)$$

In view of (2.17) and (2.19) we can easily see that

$$\widehat{\Theta}(t^{n-\frac{1}{2}}) - P_0^n \widehat{\varphi}(t^{n-\frac{1}{2}}) = (t - t^{n-\frac{1}{2}})(\Theta_t(t) - P_0^n \varphi_t(t)), \quad (4.8)$$

and thus to conclude that

$$\begin{aligned}
 \langle \widehat{\rho}_t(t), \psi \rangle + a(\rho(t), \psi) &= \ell_0^n(t) \langle (\Pi^n - I)A^{n-1}U^{n-1} - k_n^{-1}(\Pi^n - I)U^{n-1}, \psi \rangle \\
 &\quad - (t - t^{n-\frac{1}{2}}) \langle (\mathcal{R}^n - I)w_n, \psi \rangle - (t - t^{n-\frac{1}{2}}) \langle w_n - \Theta_t(t) + P_0^n \varphi_t(t), \psi \rangle \\
 &\quad - k_n^{-1} \langle (\mathcal{R}^{n-1} - I)U^{n-1} - (\mathcal{R}^n - I)U^n, \psi \rangle \\
 &\quad + \langle \xi_\Theta^n, \psi \rangle + \langle f(t) - P_0^n \widehat{\varphi}(t), \psi \rangle.
 \end{aligned} \tag{4.9}$$

□

An a posteriori error bound for the parabolic error follows. The estimate that we will derive depends still on the choice of the time reconstruction through w_n as well as on stationary finite element errors through the elliptic reconstruction \mathcal{R}^n .

Theorem 4.2. (ESTIMATES IN $L^\infty(L^2)$ AND $L^2(H^1)$ FOR THE PARABOLIC ERROR) *The following estimate is valid*

$$\max_{t \in [0, t^m]} \{ \|\widehat{\rho}(t)\|^2 + \int_0^t (|\rho(s)|_1^2 + |\widehat{\rho}(s)|_1^2) ds \} \leq \|\widehat{\rho}(0)\|^2 + \mathcal{J}_m, \tag{4.10}$$

where \mathcal{J}_m , $m = 1, \dots, N$, is defined by

$$\mathcal{J}_m := \mathcal{J}_m^{\text{T},1} + \mathcal{J}_m^{\text{T},2} + \mathcal{J}_m^{\text{S},1} + \mathcal{J}_m^{\text{S},2} + \mathcal{J}_m^{\text{C}} + \mathcal{J}_m^{\text{D}} + \mathcal{J}_m^{\text{W}}, \tag{4.11}$$

with

$$\mathcal{J}_m^{\text{T},1} := \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\sigma(s)|_1^2 ds, \tag{4.12}$$

$$\mathcal{J}_m^{\text{T},2} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle \xi_\Theta^n, \widehat{\rho}(s) \rangle| ds, \tag{4.13}$$

$$\mathcal{J}_m^{\text{S},1} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |(s - t^{n-\frac{1}{2}}) \langle (\mathcal{R}^n - I)w_n, \widehat{\rho}(s) \rangle| ds, \tag{4.14}$$

$$\mathcal{J}_m^{\text{S},2} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \left| \left\langle \frac{(\mathcal{R}^n - I)U^n - (\mathcal{R}^{n-1} - I)U^{n-1}}{k_n}, \widehat{\rho}(s) \right\rangle \right| ds, \tag{4.15}$$

$$\mathcal{J}_m^{\text{C}} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle \ell_0^n(s) (\widetilde{\Pi}^n - I)A^{n-1}U^{n-1} - k_n^{-1}(\Pi^n - I)U^{n-1}, \widehat{\rho}(s) \rangle| ds, \tag{4.16}$$

$$\mathcal{J}_m^{\text{D}} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle f(s) - P_0^n \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| ds, \tag{4.17}$$

$$\mathcal{J}_m^{\text{W}} := 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |(s - t^{n-\frac{1}{2}}) \langle w_n - \Theta_t(s) + P_0^n \varphi_t(s), \widehat{\rho}(s) \rangle| ds. \tag{4.18}$$

Proof. Setting $\psi = \widehat{\rho}$ in (4.2) and observing that

$$a(\rho(t), \widehat{\rho}(t)) = \frac{1}{2} |\rho(t)|_1^2 + \frac{1}{2} |\widehat{\rho}(t)|_1^2 - \frac{1}{2} |\widehat{\rho}(t) - \rho(t)|_1^2,$$

we obtain

$$\|\widehat{\rho}(t)\|^2 + \int_0^t (|\rho(s)|_1^2 + |\widehat{\rho}(s)|_1^2) ds \leq \|\widehat{\rho}(0)\|^2 + \int_0^t |\sigma(s)|_1^2 ds + 2 \int_0^t \langle R_n(s), \widehat{\rho}(s) \rangle ds,$$

for all $t \in [0, t^m]$. Recalling the definition (4.3) of R_n , it can be easily seen that

$$2 \int_0^{t^m} \langle R_n(s), \widehat{\rho}(s) \rangle ds \leq \mathcal{J}_m^{\text{T},2} + \mathcal{J}_m^{\text{S},1} + \mathcal{J}_m^{\text{S},2} + \mathcal{J}_m^{\text{C}} + \mathcal{J}_m^{\text{D}} + \mathcal{J}_m^{\text{W}}, \quad (4.19)$$

which completes the proof. \square

We emphasize here that the piecewise polynomial in time w_n appearing in the definition of time reconstruction (3.10) is chosen such that \mathcal{J}_m^{W} is an a posteriori quantity of optimal order. According to (3.14), the term \mathcal{J}_m^{W} vanishes in case of the time reconstruction based on one time subinterval. In addition, in case of the time reconstruction based on two adjacent time subintervals the following result is valid:

Lemma 4.3 (Calculation of $\tilde{w}_n - \Theta_t(t) + P_0^n \varphi_t(t)$). *For $t \in I_n$ we have*

$$\tilde{w}_n - \Theta_t(t) + P_0^n \varphi_t(t) = -\frac{2}{k_n + k_{n-1}} \left(z_n + \xi_\Theta^n - \pi^n \xi_\Theta^{n-1} - y_n - P_0^n \xi_\varphi^n + \pi^n P_0^{n-1} \xi_\varphi^{n-1} \right) \quad (4.20)$$

with z_n and y_n defined by

$$z_n := \frac{1}{2} \left(\frac{k_{n-1}}{k_n} A^n U^n - \left(\left(2 + \frac{k_{n-1}}{k_n} \right) \tilde{\Pi}^n - \pi^n \right) A^{n-1} U^{n-1} + \pi^n \tilde{\Pi}^{n-1} A^{n-2} U^{n-2} \right), \quad (4.21)$$

$$y_n := \frac{1}{2} \left(\frac{k_{n-1}}{k_n} P_0^n f^n - \left(\left(2 + \frac{k_{n-1}}{k_n} \right) P_0^n - \pi^n P_0^{n-1} \right) f^{n-1} + \pi^n P_0^{n-1} f^{n-2} \right).$$

Proof. We let $\tilde{\varphi}$ be given by

$$\tilde{\varphi}(t) := \ell_{1/2}^n(t) P_0^n \varphi(t^{n-\frac{1}{2}}) + \ell_{-1/2}^n(t) \pi^n P_0^{n-1} \varphi(t^{n-\frac{3}{2}}), \quad t \in I_n, \quad (4.22)$$

where

$$\ell_{1/2}^n(t) := \frac{2(t - t^{n-\frac{3}{2}})}{k_n + k_{n-1}}, \quad \ell_{-1/2}^n(t) := \frac{2(t^{n-\frac{1}{2}} - t)}{k_n + k_{n-1}}. \quad (4.23)$$

We express $\Theta(t)$, $\varphi(t)$, $t \in I_n$, defined in (2.15) and in (2.14), respectively, in terms of $\ell_{1/2}^n$ and $\ell_{-1/2}^n$, that is

$$\begin{aligned} \Theta(t) &= \ell_{1/2}^n(t) \Theta(t^{n-\frac{1}{2}}) + \ell_{-1/2}^n(t) \tilde{\Theta}^{n-\frac{3}{2}}, \quad t \in I_n, \\ \varphi(t) &= \ell_{1/2}^n(t) \varphi(t^{n-\frac{1}{2}}) + \ell_{-1/2}^n(t) \tilde{\varphi}^{n-\frac{3}{2}}, \quad t \in I_n, \end{aligned} \quad (4.24)$$

where

$$\begin{aligned} \tilde{\Theta}^{n-\frac{3}{2}} &:= \ell_0^n(t^{n-\frac{3}{2}}) \tilde{\Pi}^n A^{n-1} U^{n-1} + \ell_1^n(t^{n-\frac{3}{2}}) A^n U^n, \\ \tilde{\varphi}^{n-\frac{3}{2}} &:= \ell_0^n(t^{n-\frac{3}{2}}) \varphi(t^{n-1}) + \ell_1^n(t^{n-\frac{3}{2}}) \varphi(t^n). \end{aligned} \quad (4.25)$$

Now, in view of (3.15) and (2.21), we have

$$\begin{aligned} \tilde{w}_n - \Theta_t(t) + P_0^n \varphi_t(t) &= -\frac{2}{k_n + k_{n-1}} \left(\left[\frac{U^n - \tilde{\Pi}^n U^{n-1}}{k_n} \right] - \pi^n \left[\frac{U^{n-1} - \tilde{\Pi}^{n-1} U^{n-2}}{k_{n-1}} \right] \right) \\ &\quad - \Theta_t(t) + P_0^n \varphi_t(t) \\ &= -\frac{2}{k_n + k_{n-1}} \left(-\widehat{\Theta}(t^{n-\frac{1}{2}}) + P_0^n \widehat{\varphi}(t^{n-\frac{1}{2}}) - \pi^n [-\widehat{\Theta}(t^{n-\frac{3}{2}}) + P_0^n \widehat{\varphi}(t^{n-\frac{3}{2}})] \right) \\ &\quad + \Theta(t^{n-\frac{1}{2}}) - \tilde{\Theta}^{n-\frac{3}{2}} - P_0^n \varphi(t^{n-\frac{1}{2}}) + P_0^n \tilde{\varphi}^{n-\frac{3}{2}}. \end{aligned}$$

According to (2.17) and (2.19), we get

$$\begin{aligned} \tilde{w}_n - \Theta_t(t) + P_0^n \varphi_t(t) &= -\frac{2}{k_n + k_{n-1}} \left(\pi^n \Theta(t^{n-\frac{3}{2}}) - \tilde{\Theta}^{n-\frac{3}{2}} + \xi_\Theta^n - \pi^n \xi_\Theta^{n-1} \right. \\ &\quad \left. - \pi^n P_0^{n-1} \varphi(t^{n-\frac{3}{2}}) + P_0^n \tilde{\varphi}^{n-\frac{3}{2}} - P_0^n \xi_\varphi^n + \pi^n P_0^{n-1} \xi_\varphi^{n-1} \right), \quad t \in I_n. \end{aligned} \quad (4.26)$$

In view of (2.15), (4.25) and (4.21), we can easily see that

$$\pi^n \Theta(t^{n-\frac{3}{2}}) - \tilde{\Theta}^{n-\frac{3}{2}} = z_n \quad \text{and} \quad \pi^n P_0^n \varphi(t^{n-\frac{3}{2}}) - P_0^n \tilde{\varphi}^{n-\frac{3}{2}} = y_n, \quad (4.27)$$

and the desired result follows. \square

Next, we shall further investigate each term of the estimator by considering both time reconstructions in combination with residual-based a posteriori estimators for the elliptic error; other choices of estimators for the stationary finite element errors are also possible.

4.2. A residual-based a posteriori bound for the parabolic error. In this paragraph we use the space-time reconstruction introduced in (3.17), with w_n to be chosen either as in (3.14) or as in (3.15), and residual-based estimators to derive an upper bound for the parabolic error $\hat{\rho}$. The proof is split in several steps.

Throughout the rest of this paragraph we denote by $t_\star^m \in [0, t^m]$ a point for which

$$\|\hat{\rho}(t_\star^m)\| = \max_{t \in [0, t^m]} \|\hat{\rho}(t)\|. \quad (4.28)$$

We shall first state an upper bound for the terms $\mathcal{J}_m^{\text{T},1}$ and $\mathcal{J}_m^{\text{T},2}$ appearing in Theorem 4.2, which measure the local time discretisation error. Note that the estimate for $\mathcal{J}_m^{\text{T},1}$ has been proved in Lemma 3.19 and the estimate for $\mathcal{J}_m^{\text{T},2}$ can be easily seen.

Lemma 4.4 (Time error estimate). *Let $v_n \in \mathbb{V}^n$ and the time estimator $\mathcal{E}_m^{\text{T},2}$ be defined as follows*

$$\mathcal{E}_m^{\text{T},2} := 2 \sum_{n=1}^m k_n \|\xi_\Theta^n\|. \quad (4.29)$$

Then, we have

$$\mathcal{J}_m^{\text{T},1} \leq (\mathcal{E}_{1,m}^{\text{rec}}(w_n))^2 \quad \text{or} \quad \mathcal{J}_m^{\text{T},1} \leq (\mathcal{E}_{1,m}^{\text{rec}}(\tilde{w}_n))^2, \quad (4.30)$$

depending on the choice of the time reconstruction with w_n and \tilde{w}_n as defined in (3.14) and (3.15), respectively. In addition, the term $\mathcal{J}_m^{\text{T},2}$ may be bounded as follows

$$\mathcal{J}_m^{\text{T},2} \leq \|\hat{\rho}(t_\star^m)\| \mathcal{E}_m^{\text{T},2}. \quad (4.31)$$

We shall next estimate the term $\mathcal{J}_m^{\text{S},1}$ in Theorem 4.2 which accounts for the space discretisation error.

Lemma 4.5 (Spatial error estimate). *Let $v_n \in \mathbb{V}^n$ and $\mathcal{E}_m^{\text{S},1}$ be defined as*

$$\mathcal{E}_m^{\text{S},1}(v_n) := \sum_{n=1}^m \frac{k_n^2}{2} \eta_n(v_n).$$

Then, depending on the choice of the time reconstruction, the following estimate is valid

$$\mathcal{J}_m^{\text{S},1} \leq \|\hat{\rho}(t_\star^m)\| \mathcal{E}_m^{\text{S},1}(w_n) \quad \text{or} \quad \mathcal{J}_m^{\text{S},1} \leq \|\hat{\rho}(t_\star^m)\| \mathcal{E}_m^{\text{S},1}(\tilde{w}_n), \quad (4.32)$$

where w_n and \tilde{w}_n are defined in (3.14) and (3.15), respectively.

Proof. Since w_n is piecewise constant in time, we can easily see that

$$\int_{t^{n-1}}^{t^n} |(s - t^{n-\frac{1}{2}}) \langle (\mathcal{R}^n - I)w_n, \widehat{\rho}(s) \rangle| ds \leq \frac{k_n^2}{4} \max_{t \in [t^{n-1}, t^n]} \|\widehat{\rho}(t)\| \|(\mathcal{R}^n - I)w_n\| \quad (4.33)$$

and the desired result follows. \square

An upper bound for the term $\mathcal{J}_m^{\text{S},2}$ in Theorem 4.2 will be presented next.

Lemma 4.6 (Space estimator accounting for mesh changing). *Let $\mathcal{E}_m^{\text{S},2}$ be defined as*

$$\mathcal{E}_m^{\text{S},2} := 2 \sum_{n=1}^m k_n \delta_n \quad (4.34)$$

with

$$\begin{aligned} \delta_n := & (C_{1,2} \|\check{h}_n^2 (k_n^{-1} (\text{div}(\mathbf{A}\nabla) + A^n)U^n - k_n^{-1} (\text{div}(\mathbf{A}\nabla) + A^{n-1})U^{n-1})\|_{\check{T}_n} \\ & + C_{2,2} \|\check{h}_n^{3/2} J[\mathbf{A}\nabla U^n - \mathbf{A}\nabla U^{n-1}]\|_{\check{\Sigma}_n}). \end{aligned} \quad (4.35)$$

Then, we have

$$\mathcal{J}_m^{\text{S},2} \leq \|\widehat{\rho}(t_\star^m)\| \mathcal{E}_m^{\text{S},2}. \quad (4.36)$$

Proof. Let $z : [0, T] \rightarrow H_0^1$ be the solution of problem

$$a(\chi, z(t)) = \langle \widehat{\rho}(t), \chi \rangle, \quad \forall \chi \in H_0^1, \quad t \in [0, T], \quad (4.37)$$

and $\widehat{\mathcal{I}}^n z(t) \in \mathbb{V}^n \cap \mathbb{V}^{n-1}$, $t \in I_n$, be its Clément-type interpolant. Since $\widehat{\mathcal{I}}^n z(t) \in \mathbb{V}^n \cap \mathbb{V}^{n-1}$, using first (4.37), the orthogonality property of the elliptic reconstruction (3.2) in $\mathbb{V}^{n-1} \cap \mathbb{V}^n$, and integration by parts, we get

$$\begin{aligned} & \langle (\mathcal{R}^n - I)U^n - (\mathcal{R}^{n-1} - I)U^{n-1}, \widehat{\rho}(t) \rangle \\ &= a((\mathcal{R}^n - I)U^n - (\mathcal{R}^{n-1} - I)U^{n-1}, (z - \widehat{\mathcal{I}}^n z)(t)) \\ &= \sum_{K \in \check{T}_n} \int_K ((\text{div}(\mathbf{A}\nabla) + A^n)U^n - (\text{div}(\mathbf{A}\nabla) + A^{n-1})U^{n-1})(z - \widehat{\mathcal{I}}^n z)(t) \\ & \quad - \sum_{e \in \check{\Sigma}_n} \int_e J[\mathbf{A}\nabla U^n - \mathbf{A}\nabla U^{n-1}](z - \widehat{\mathcal{I}}^n z)(t). \end{aligned} \quad (4.38)$$

Hence, in view of (2.9), we obtain

$$\begin{aligned} & \sum_{K \in \check{T}_n} \int_K ((\text{div}(\mathbf{A}\nabla) + A^n)U^n - (\text{div}(\mathbf{A}\nabla) + A^{n-1})U^{n-1})(z - \widehat{\mathcal{I}}^n z)(t) \\ & \leq C_{1,2} \|\check{h}_n^2 ((\text{div}(\mathbf{A}\nabla) + A^n)U^n - (\text{div}(\mathbf{A}\nabla) + A^{n-1})U^{n-1})\| \|\widehat{\rho}(t)\|, \end{aligned} \quad (4.39)$$

and

$$\sum_{e \in \check{\Sigma}_n} \int_e J[\mathbf{A}\nabla U^n - \mathbf{A}\nabla U^{n-1}](z - \widehat{\mathcal{I}}^n z)(t) \leq C_{2,2} \|\check{h}_n^{3/2} J[\mathbf{A}\nabla U^n - \mathbf{A}\nabla U^{n-1}]\|_{\check{\Sigma}_n} \|\widehat{\rho}(t)\|; \quad (4.40)$$

the claimed result follows. \square

We can easily see that the term \mathcal{J}_m^{C} in Theorem 4.2 corresponding to the coarsening error can be bounded as follows

Lemma 4.7 (Coarsening error estimate). *Let \mathcal{E}_m^C be the coarsening estimator defined by*

$$\mathcal{E}_m^C := 2 \sum_{n=1}^m k_n \beta_n \quad \text{with} \quad \beta_n := \|(I^n - I)(A^{n-1}U^{n-1} + k_n^{-1}U^{n-1})\|_{\mathcal{T}_n}. \quad (4.41)$$

Then, it holds

$$\mathcal{J}_m^C \leq \|\widehat{\rho}(t_\star^m)\| \mathcal{E}_m^C. \quad (4.42)$$

Upper bounds for the term \mathcal{J}_m^D which measure the data approximation error, will be shown in the next lemma.

Lemma 4.8 (Data error estimate). *Let*

$$\begin{aligned} \zeta_{n,1} &:= \frac{1}{k_n} \int_{t^{n-1}}^{t^n} \|f(s) - \varphi(s)\| ds, \\ \zeta_{n,2} &:= c_{1,1} \max\{\|h_n(I - P_0^n)(f^{n-1} + \xi_\varphi^n)\|, \|h_n(I - P_0^n)(f^n + \xi_\varphi^n)\|\}, \end{aligned} \quad (4.43)$$

and

$$\mathcal{E}_m^{D,1} := 2 \sum_{n=1}^m k_n (\zeta_{n,1} + \|\xi_\varphi^n\|) \quad (4.44)$$

with ξ_φ^n defined in (2.20). Then, we have

$$\mathcal{J}_m^{D,2} \leq \|\widehat{\rho}(t_\star^m)\| \mathcal{E}_m^{D,1} + 2 \sum_{n=1}^m \left(\int_{t^{n-1}}^{t^n} |\widehat{\rho}(s)|^2 \right)^{1/2} k_n^{1/2} \zeta_{n,2}. \quad (4.45)$$

Proof. The term $\mathcal{J}_m^{D,2}$ may be bounded as follows

$$\begin{aligned} \mathcal{J}_m^{D,2} &= 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle f(s) - P_0^n \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| ds \\ &\leq 2 \sum_{n=1}^m \int_{t^{n-1}}^{t^n} \{|\langle f(s) - \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| + |\langle (I - P_0^n) \widehat{\varphi}(s), \widehat{\rho}(s) \rangle|\} ds. \end{aligned} \quad (4.46)$$

Now, we have

$$\int_{t^{n-1}}^{t^n} |\langle f(s) - \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| ds \leq \max_{t \in [t^{n-1}, t^n]} \|\rho(t)\| \int_{t^{n-1}}^{t^n} \{\|f(s) - \varphi(s)\| + \|\xi_\varphi^n\|\} ds,$$

from which we can conclude that

$$\sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle f(s) - \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| ds \leq \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m k_n (\zeta_{n,1} + \|\xi_\varphi^n\|). \quad (4.47)$$

Furthermore, using again the orthogonality property of P_0^n , we obtain

$$\langle (I - P_0^n) \widehat{\varphi}(s), \widehat{\rho}(s) \rangle = \langle (I - P_0^n) \widehat{\varphi}(s), (\widehat{\rho} - \mathcal{I}^n \widehat{\rho})(s) \rangle \leq c_{1,1} \|h_n(I - P_0^n) \widehat{\varphi}(s)\| |\widehat{\rho}(s)|_1.$$

Now,

$$\begin{aligned} \|h_n(I - P_0^n) \widehat{\varphi}(s)\| &= \|h_n(I - P_0^n)[\ell_0^n(s)f^{n-1} + \ell_1^n(s)f^n + \xi_\varphi^n]\| \\ &\leq \max\{\|h_n(I - P_0^n)(f^{n-1} + \xi_\varphi^n)\|, \|h_n(I - P_0^n)(f^n + \xi_\varphi^n)\|\}, \end{aligned}$$

and hence,

$$\sum_{n=1}^m \int_{t^{n-1}}^{t^n} |\langle (I - P_0^n) \widehat{\varphi}(s), \widehat{\rho}(s) \rangle| ds \leq \sum_{n=1}^m c_{1,1} \left(\int_{t^{n-1}}^{t^n} |\widehat{\rho}(s)|^2 \right)^{1/2} k_n^{1/2} \zeta_{n,2}. \quad (4.48)$$

In view of (4.47), (4.48), we conclude the desired result. \square

Lemma 4.9 (An estimator for \mathcal{J}_m^W). *The term \mathcal{J}_m^W vanishes in case of the two time-level reconstruction. Furthermore, the term \mathcal{J}_m^W corresponding to the three time-level reconstruction may be bounded as follows*

$$\begin{aligned} \mathcal{J}_m^W &\leq \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m \frac{k_n^2}{2(k_n + k_{n-1})} \|z_n\| + \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m \frac{k_n^2}{4} (\|\xi_\Theta^n\| + \|\pi^n \xi_\Theta^{n-1}\|) \\ &+ \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m \frac{k_n^2}{2(k_n + k_{n-1})} \|y_n\| + \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m \frac{k_n^2}{4} (\|P_0^n \xi_\varphi^n\| + \|\pi^n P_0^{n-1} \xi_\varphi^{n-1}\|) \end{aligned} \quad (4.49)$$

with z_n and y_n as defined in (4.21).

Proof. According to (4.20), the term \mathcal{J}_m^W may be bounded as follows

$$\begin{aligned} \mathcal{J}_m^W &\leq \sum_{n=1}^m \frac{2}{k_n + k_{n-1}} \int_{t^{n-1}}^{t^n} |s - t^{n-\frac{1}{2}}| (|\langle z_n, \widehat{\rho}(s) \rangle| + |\langle y_n, \widehat{\rho}(s) \rangle|) ds \\ &+ \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |s - t^{n-\frac{1}{2}}| (|\langle \xi_\Theta^n, \widehat{\rho}(s) \rangle| + |\langle \pi^n \xi_\Theta^{n-1}, \widehat{\rho}(s) \rangle|) ds \\ &+ \sum_{n=1}^m \int_{t^{n-1}}^{t^n} |s - t^{n-\frac{1}{2}}| (|\langle P_0^n \xi_\varphi^n, \widehat{\rho}(s) \rangle| + |\langle \pi^n P_0^{n-1} \xi_\varphi^{n-1}, \widehat{\rho}(s) \rangle|) ds, \end{aligned} \quad (4.50)$$

and the claimed result follows. \square

We can thus conclude the following a posteriori estimates for the parabolic error:

Lemma 4.10 (An $L^\infty(L^2)$ a posteriori error bound for $\widehat{\rho}$ — two time-level reconstruction). *For $m = 1, \dots, N$, the following estimate holds*

$$\begin{aligned} \max_{t \in [0, t^m]} \|\widehat{\rho}(t)\| + \left(\int_0^{t^m} |\widehat{\rho}(s)|_1^2 ds \right)^{1/2} &\leq \sqrt{2} \|\widehat{\rho}(0)\| + \mathcal{E}_m^{T,1}(w_n) \\ &+ \left((\mathcal{E}_m^{T,2} + \mathcal{E}_m^{S,1}(w_n) + \mathcal{E}_m^{S,2} + \mathcal{E}_m^C + \mathcal{E}_m^{D,1})^2 + (\mathcal{E}_m^{D,2})^2 \right)^{1/2}, \end{aligned} \quad (4.51)$$

where

$$\mathcal{E}_m^{D,2} := \sum_{n=1}^m k_n^{1/2} \zeta_{n,2} \quad (4.52)$$

and $\zeta_{n,2}$ as defined in (4.43).

Proof. In view of Theorem 4.2, we can easily see that

$$\|\widehat{\rho}(t_\star^m)\|^2 + \int_0^{t^m} |\widehat{\rho}(s)|_1^2 ds \leq 2 \|\widehat{\rho}(0)\|^2 + 2 \mathcal{J}_m. \quad (4.53)$$

Thus, by making use of the previous lemmas, we can conclude that

$$\begin{aligned}
\|\widehat{\rho}(t_\star^m)\|^2 + \int_0^{t^m} |\widehat{\rho}(s)|_1^2 ds &\leq 2 \|\widehat{\rho}(0)\|^2 + 2 \sum_{n=1}^m k_n \gamma_n^2(w_n) \\
&+ 4 \|\widehat{\rho}(t_\star^m)\| \sum_{n=1}^m k_n (\|\xi_\Theta^n\| + k_n \eta_n(w_n) + \delta_n + \beta_n + \zeta_{n,1} + \|\xi_\varphi^n\|) \\
&+ 4 \sum_{n=1}^m \left(\int_{t^{n-1}}^{t^n} |\widehat{\rho}(s)|_1^2 ds \right)^{1/2} k_n^{1/2} \zeta_{n,2}.
\end{aligned} \tag{4.54}$$

The final estimate is derived by using the following fact: Let $c \in \mathbb{R}$ and $\mathbf{a} = (a_0, a_1, \dots, a_m)$, $\mathbf{b} = (b_0, b_1, \dots, b_m) \in \mathbb{R}^{m+1}$ be such that $|\mathbf{a}|^2 \leq c^2 + \mathbf{a} \cdot \mathbf{b}$, then $|\mathbf{a}| \leq |c| + |\mathbf{b}|$, cf. [21]. Indeed, we apply the above result to the case

$$\begin{aligned}
c &= \left(2 \|\widehat{\rho}(0)\|^2 + 2 \sum_{n=1}^m k_n \gamma_n^2(w_n) \right)^{1/2}, \\
a_0 &= \|\widehat{\rho}(t_\star^m)\|, \quad a_n = \left(\int_{t^{n-1}}^{t^n} |\widehat{\rho}(s)|_1^2 ds \right)^{1/2}, \quad n = 1, \dots, m, \\
b_0 &= 4 \sum_{n=1}^m k_n (\|\xi_\Theta^n\| + k_n \eta_n(w_n) + \delta_n + \beta_n + \zeta_{n,1} + \|\xi_\varphi^n\|) \\
b_n &= 4 k_n^{1/2} \zeta_{n,2}, \quad n = 1, \dots, m,
\end{aligned}$$

to get the final estimate. □

The analogue of Lemma 4.10 in the case of the three time-level reconstruction follows

Lemma 4.11 (An $L^\infty(L^2)$ a posteriori error bound for $\widehat{\rho}$ — three time-level reconstruction).
For $m = 1, \dots, N$, the following estimate holds

$$\begin{aligned}
\max_{t \in [0, t^m]} \|\widehat{\rho}(t)\| + \left(\int_0^{t^m} |\widehat{\rho}(s)|_1^2 ds \right)^{1/2} &\leq \sqrt{2} \|\widehat{\rho}(0)\| + \mathcal{E}_m^{\text{T},1}(\tilde{w}_n) + \left((\mathcal{E}_m^{\text{T},2} + \mathcal{E}_m^{\text{T},3}) \right. \\
&\left. + \mathcal{E}_m^{\text{S},1}(\tilde{w}_n) + \mathcal{E}_m^{\text{S},2} + \mathcal{E}_m^{\text{C}} + \mathcal{E}_m^{\text{D},1} + \mathcal{E}_{m,1} \right)^2 + (\mathcal{E}_m^{\text{D},2})^2)^{1/2},
\end{aligned} \tag{4.55}$$

where

$$\begin{aligned}
\mathcal{E}_m^{\text{T},3} &:= \sum_{n=1}^m \frac{k_n^2}{2(k_n + k_{n-1})} \|z_n\| \\
\mathcal{E}_{m,1} &:= \sum_{n=1}^m k_n \left(\frac{k_n}{2(k_n + k_{n-1})} \|y_n\| + \frac{k_n}{4} (\|\xi_\Theta^n\| + \|\pi^n \xi_\Theta^{n-1}\|) \right. \\
&\quad \left. + \frac{k_n}{4} (\|P_0^n \xi_\varphi^n\| + \|\pi^n P_0^{n-1} \xi_\varphi^{n-1}\|) \right).
\end{aligned} \tag{4.56}$$

By appropriately combining the results from §3.5 and §§4.1-4.2 we can conclude the main results of this paragraph, which are stated in the next two theorems.

Theorem 4.12 ($L^\infty(L^2)$ and $L^2(H^1)$ a posteriori error estimates based on one time subinterval).
For $m = 1, \dots, N$, the following estimates hold

$$\begin{aligned}
\max_{t \in [0, t^m]} \|u(t) - U(t)\| &\leq \sqrt{2} \|u^0 - \mathcal{R}^0 u^0\| + \mathcal{E}_m^{\text{T},1}(w_n) + \left((\mathcal{E}_m^{\text{T},2} + \mathcal{E}_m^{\text{S},1}(w_n)) \right. \\
&\quad \left. + \mathcal{E}_m^{\text{S},2} + \mathcal{E}_m^{\text{S}} + \mathcal{E}_m^{\text{D},1} \right)^2 + (\mathcal{E}_m^{\text{D},2})^2)^{1/2} + \mathcal{E}_{2,m}^{\text{rec}}(w_n) + \mathcal{E}_{2,m}^{\text{ell}}.
\end{aligned} \tag{4.57}$$

$$\begin{aligned} \left(\int_0^{t^m} |u(t) - U(t)|_1^2 \right)^{1/2} &\leq \sqrt{2} \|u^0 - \mathcal{R}^0 u^0\| + \mathcal{E}_m^{\text{T},1}(w_n) + \left((\mathcal{E}_m^{\text{T},2} + \mathcal{E}_m^{\text{S},1}(w_n) \right. \\ &\quad \left. + \mathcal{E}_m^{\text{S},2} + \mathcal{E}_m^{\text{C}} + \mathcal{E}_m^{\text{D},1})^2 + (\mathcal{E}_m^{\text{D},2})^2 \right)^{1/2} + \mathcal{E}_{1,m}^{\text{rec}}(w_n) + \mathcal{E}_{1,m}^{\text{ell}}. \end{aligned} \quad (4.58)$$

Theorem 4.13 ($L^\infty(L^2)$ and $L^2(H^1)$ a posteriori error estimates based on two adjacent time intervals). *For $m = 1, \dots, N$, the following estimates hold*

$$\begin{aligned} \max_{t \in [0, t^m]} \|u(t) - U(t)\| &\leq \sqrt{2} \|u^0 - \mathcal{R}^0 u^0\| + \mathcal{E}_m^{\text{T},1}(\tilde{w}_n) + \left((\mathcal{E}_m^{\text{T},2} + \mathcal{E}_m^{\text{T},3} + \mathcal{E}_m^{\text{S},1}(\tilde{w}_n) \right. \\ &\quad \left. + \mathcal{E}_m^{\text{S},2} + \mathcal{E}_m^{\text{C}} + \mathcal{E}_m^{\text{D},1} + \mathcal{E}_{m,1})^2 + (\mathcal{E}_m^{\text{D},2})^2 \right)^{1/2} + \mathcal{E}_{2,m}^{\text{rec}}(\tilde{w}_n) + \mathcal{E}_{2,m}^{\text{ell}}. \end{aligned} \quad (4.59)$$

$$\begin{aligned} \left(\int_0^{t^m} |u(t) - U(t)|_1^2 \right)^{1/2} &\leq \sqrt{2} \|u^0 - \mathcal{R}^0 u^0\| + \mathcal{E}_m^{\text{T},1}(\tilde{w}_n) + \left((\mathcal{E}_m^{\text{T},2} + \mathcal{E}_m^{\text{T},3} + \mathcal{E}_m^{\text{S},1}(\tilde{w}_n) \right. \\ &\quad \left. + \mathcal{E}_m^{\text{S},2} + \mathcal{E}_m^{\text{C}} + \mathcal{E}_m^{\text{D},1} + \mathcal{E}_{m,1})^2 + (\mathcal{E}_m^{\text{D},2})^2 \right)^{1/2} + \mathcal{E}_{1,m}^{\text{rec}}(\tilde{w}_n) + \mathcal{E}_{1,m}^{\text{ell}}. \end{aligned} \quad (4.60)$$

5. ASYMPTOTIC BEHAVIOUR OF THE ESTIMATORS

In this section we compare the error estimators with the true error and study their asymptotic behaviour. For the implementation of the estimators we used the adaptive finite element library ALBERTA-FEM [32].

For our purpose, we consider the linear parabolic equation with $a_{ij} \equiv \delta_{ij}$, i.e., the heat equation, on the unit square $\Omega = [0, 1]^2$, $T = 1$, and the exact solution u be one of the following:

- case (1): $u(x, y, t) = \sin(\pi t) \sin(\pi x) \sin(\pi y)$,
- case (2): $u(x, y, t) = \sin(15\pi t) \sin(\pi x) \sin(\pi y)$ (faster oscillations in time),
- case (3): $u(x, y, t) = \sin(0.5\pi t) \sin(10\pi x) \sin(10\pi y)$ (faster oscillations in space),
- case (4): $u(x, y, t) = t^2 \sin((x^2 - x)(y^2 - y))$.

The boundary and initial conditions are exactly zero in all cases and the right-hand side f is calculated by applying the linear parabolic operator to each u .

We conduct tests on uniform meshes with uniform time steps. For the discretisation in space we use linear Lagrange elements. For $m = 1, \dots, N$, we compute the quantities: the *error in the discrete $L^\infty(0, t^m; L^2(\Omega))$ -norm*

$$\max_{0 \leq n \leq m} \|e^n\| = \max_{0 \leq n \leq m} \|u(t^n) - U^n\|,$$

the *total error*, which is dominated by the discrete $L^2(0, t^m; H^1(\Omega))$ error,

$$e_{\text{total}}(t^m) := \max_{0 \leq n \leq m} \left(\|e^n\|^2 + \sum_{n=1}^m k_n \|\nabla e^n\|^2 \right)^{1/2},$$

the elliptic reconstruction estimator $\mathcal{E}_{2,m}^{\text{ell}}$ and the time reconstruction estimators $\mathcal{E}_{2,m}^{\text{rec}}(w_n)$, $\mathcal{E}_{2,m}^{\text{rec}}(\tilde{w}_n)$ introduced in Section 3.5, the time estimators $\mathcal{E}_m^{\text{T},1}(w_n)$, $\mathcal{E}_m^{\text{T},1}(\tilde{w}_n)$, $\mathcal{E}_m^{\text{T},2}$, $\mathcal{E}_m^{\text{T},3}$ and the space estimators $\mathcal{E}_m^{\text{S},1}(w_n)$, $\mathcal{E}_m^{\text{S},1}(\tilde{w}_n)$, $\mathcal{E}_m^{\text{S},2}$ introduced in Section 4.2. We exclude from the numerical experiments the coarsening error estimator \mathcal{E}_N^{C} that vanishes as well as the terms corresponding to the approximation of data u^0 and f which clearly are of optimal order and thus do not contain interesting information for our purposes.

Moreover, for $1 \leq m \leq N$, we calculate the following quantities:

- the *total time estimators*

$$\begin{aligned}\mathcal{E}_m^T(w_n) &= \mathcal{E}_m^{T,1}(w_n) + \mathcal{E}_m^{T,2} + \mathcal{E}_{2,m}^{\text{rec}}(w_n), \\ \mathcal{E}_m^T(\tilde{w}_n) &= \mathcal{E}_m^{T,1}(\tilde{w}_n) + \mathcal{E}_m^{T,2} + \mathcal{E}_m^{T,3} + \mathcal{E}_{2,m}^{\text{rec}}(\tilde{w}_n),\end{aligned}$$

- the *total space estimators*

$$\mathcal{E}_m^S(w_n) = \mathcal{E}_m^{S,1}(w_n) + \mathcal{E}_m^{S,2} + \mathcal{E}_{2,m}^{\text{ell}} \quad \text{and} \quad \mathcal{E}_m^S(\tilde{w}_n) = \mathcal{E}_m^{S,1}(\tilde{w}_n) + \mathcal{E}_m^{S,2} + \mathcal{E}_{2,m}^{\text{ell}},$$

- and the *total estimators*

$$\mathcal{E}_m = \mathcal{E}_m^T(w_n) + \mathcal{E}_m^S(w_n) \quad \text{and} \quad \tilde{\mathcal{E}}_m := \mathcal{E}_m^T(\tilde{w}_n) + \mathcal{E}_m^S(\tilde{w}_n).$$

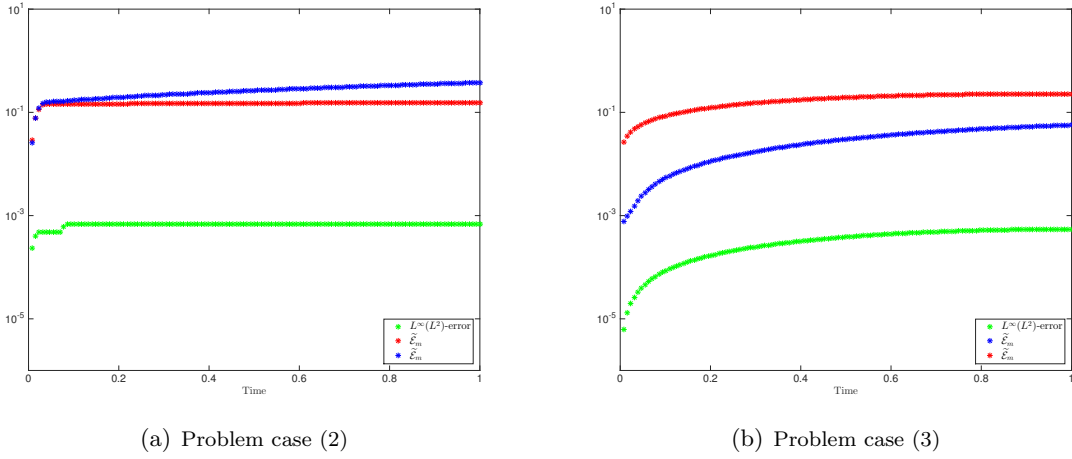


FIGURE 1. The $L^\infty(0, t^m, L^2(\Omega))$ -error and the two-level and three-level estimators \mathcal{E}_m and $\tilde{\mathcal{E}}_m$, respectively (in logarithmic scale).

Furthermore, for all quantities of interest we look at their experimental order of convergence (EOC). The EOC is defined as follows: for a given finite sequence of successive runs (indexed by i), the EOC of the corresponding sequence of quantities of interest $E(i)$ (error or estimator), is itself a sequence defined by

$$\text{EOC}(E(i)) := \frac{\log(E(i+1)/E(i))}{\log(h(i+1)/h(i))},$$

where $h(i)$ denotes the mesh-size of the run i . The values of EOC of a given quantity indicates its order.

Since the finite element spaces consist of linear Lagrange elements and the fractional-step ϑ -scheme is second-order accurate, we expect the error in $L^\infty(0, t^m, L^2(\Omega))$ to be $O(k^2 + h^2)$ and the error in $L^2(0, t^m, H^1(\Omega))$ to be $O(k^2 + h)$, where h and k denote the mesh-size and the time-step, respectively. We note here that, in order to show the optimality of the $L^\infty(0, t^m, L^2(\Omega))$ error norm and of the corresponding estimators, that is EOC 2, in each run we take $h = k$.

We are also interested in computing the corresponding effectivity indices that are defined as the ratio between the total a posteriori error estimator and the corresponding error norm, namely

$$\text{EI}(t^m) := \frac{\mathcal{E}_m}{\max_{0 \leq n \leq m} \|e^n\|} \quad \text{and} \quad \tilde{\text{EI}}(t^m) := \frac{\tilde{\mathcal{E}}_m}{\max_{0 \leq n \leq m} \|e^n\|}, \quad 1 \leq m \leq N.$$

The main conclusion of this paragraph is that all error estimators, in both cases of time reconstruction, decrease with at least second order with respect to temporal and spatial variable, Tables 1-8. Note that the space estimators $E_m^{S,1}(w_n), E_m^{S,1}(\tilde{w}_n)$ super-converge. The results listed in Table 1 and Table 5 show that all effectivity indices are asymptotically constant and, particularly, the effectivity indices $\widetilde{\text{EI}}$ corresponding to the one-time level reconstruction are smaller than the effectivity indices $\widetilde{\text{EI}}$ corresponding to the two-time level reconstruction.

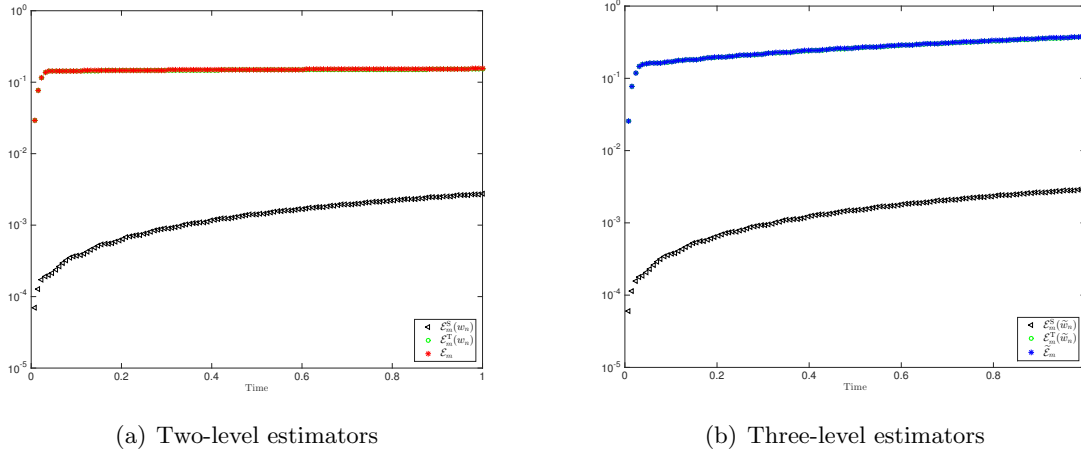


FIGURE 2. Problem case (2): The two-level estimators $\mathcal{E}_m^T(w_n)$, $\mathcal{E}_m^S(w_n)$ and \mathcal{E}_m and the three-level estimators $\mathcal{E}_m^T(\tilde{w}_n)$, $\mathcal{E}_m^S(\tilde{w}_n)$ and $\tilde{\mathcal{E}}_m$ (in logarithmic scale).

We observe that, in case of a problem with a fast time-oscillating exact solution, the two-level and three-level total time estimators are almost equal and dominate the corresponding total space estimators, which seem to be equal (Figure 2). Indeed, all the time estimators are greater than the space estimators, the time estimators $\mathcal{E}_m^{T,2}$ and $\mathcal{E}_m^{T,3}$ are almost equal and dominate all other time estimators (Figure 3). However, in case of a problem with a fast space-oscillating exact solution we observe a different behaviour and, particularly, the three-level total time estimator is smaller than the two-level total time estimator (Figure 4). Specifically, the time estimator $\mathcal{E}_m^T(w_n)$ dominates all other time estimators as well as all space estimators corresponding to both reconstructions (Figure 5). Although the main contribution to $\mathcal{E}_m^T(w_n)$ is $\mathcal{E}_m^{T,1}(w_n)$, the estimators $\mathcal{E}_m^{T,2}, \mathcal{E}_m^{T,3}$ contribute mainly to $\mathcal{E}_m^T(\tilde{w}_n)$. Regarding the space estimators, in case of the two-level reconstruction $\mathcal{E}_m^{S,1}(w_n)$ dominates $\mathcal{E}_m^{\text{ell}}$ and $\mathcal{E}_m^{S,2}$, and in case of the three-level reconstruction $\mathcal{E}_m^{S,1}(\tilde{w}_n)$ is dominated by $\mathcal{E}_m^{\text{ell}}$ and $\mathcal{E}_m^{S,2}$ (Figure 5). We can thus conclude that in a posteriori estimators equivalent terms in order corresponding to discrete derivatives (e.g., $\mathcal{E}_m^{S,1}(w_n)$ and $\mathcal{E}_m^{S,1}(\tilde{w}_n)$) may behave differently.

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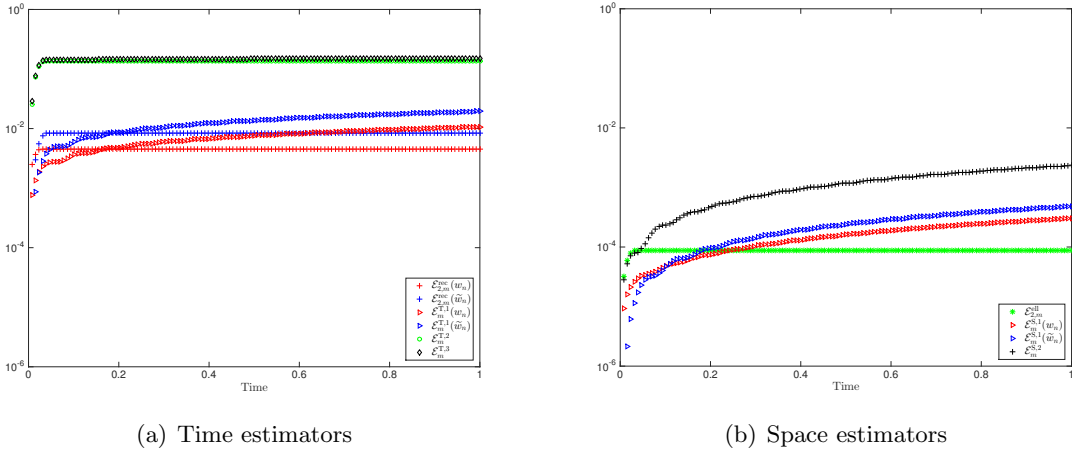


FIGURE 3. Problem case (2): The two-level and three-level estimators (in logarithmic scale).

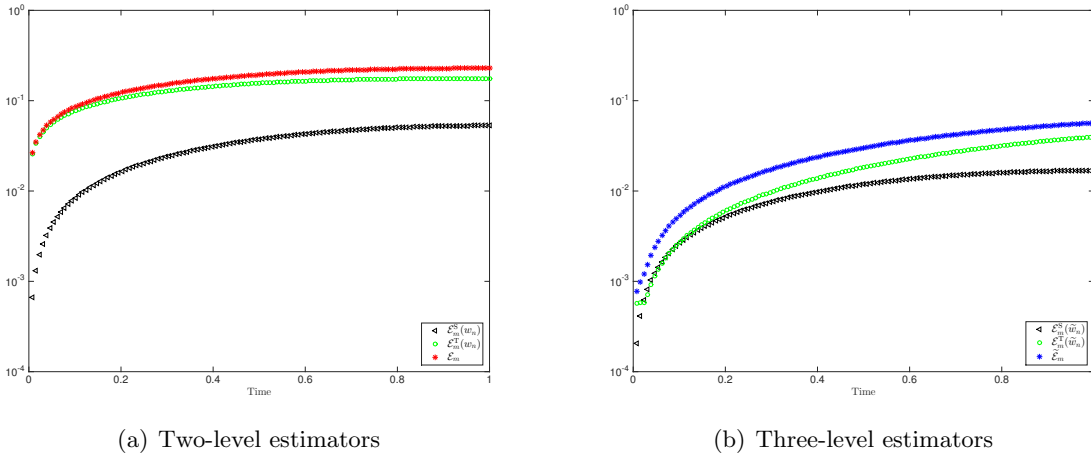


FIGURE 4. Problem case (3): The two-level estimators $\mathcal{E}_m^T(w_n)$, $\mathcal{E}_m^S(w_n)$ and \mathcal{E}_m and the three-level estimators $\mathcal{E}_m^T(\tilde{w}_n)$, $\mathcal{E}_m^S(\tilde{w}_n)$ and $\tilde{\mathcal{E}}_m$ (in logarithmic scale).

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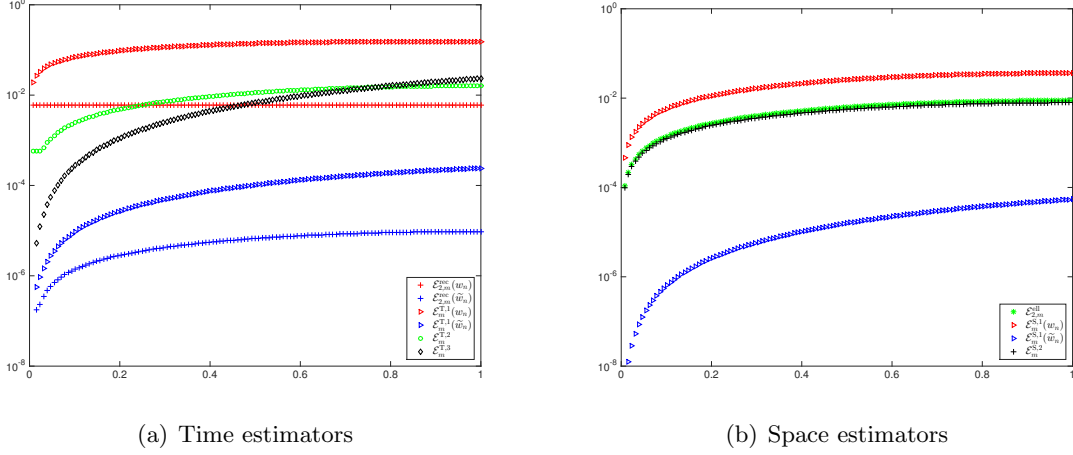


FIGURE 5. Problem case (3): The two-level and three-level estimators (in logarithmic scale).

Errors and Total Estimators

$h = k$	$\max_n \ e^n\ $	EOC	$e_{\text{total}}(t^N)$	EOC	\mathcal{E}_N	$\text{EI}(t^N)$	$\tilde{\mathcal{E}}_N$	$\tilde{\text{EI}}(t^N)$
1.2500e-01	1.4481e-03		3.7925e-02		3.6810e-01	254	4.9986e-01	345
6.2500e-02	3.4561e-04	2.04	1.8534e-02	1.03	8.6375e-02	249	1.2473e-01	360
3.1250e-02	8.4256e-05	2.02	9.1731e-03	1.01	2.0828e-02	247	3.1030e-02	368
1.5625e-02	2.0821e-05	2.01	4.5645e-03	1.00	4.7780e-03	229	7.7309e-03	371
7.8125e-03	5.1718e-06	2.00	2.2769e-03	1.00	1.1813e-03	228	1.9289e-03	372

TABLE 1. Problem case (1): the $L^\infty(0, 1; L^2(\Omega))$ -error, the total error $e_{\text{total}}(t^N)$, and the corresponding EOCs, the two- and three-level estimators \mathcal{E}_N and $\tilde{\mathcal{E}}_N$, respectively, and the corresponding effectivity indices $\text{EI}(t^N)$ and $\tilde{\text{EI}}(t^N)$.

Reconstruction Error Estimators

$h = k$	$\mathcal{E}_{2,N}^{\text{ell}}$	EOC	$\mathcal{E}_{2,N}^{\text{rec}}(w_n)$	EOC	$\mathcal{E}_{2,N}^{\text{rec}}(\tilde{w}_n)$	EOC
1.2500e-01	2.2702e-02		3.2184e-02		9.9205e-03	
6.2500e-02	5.6786e-03	1.99	7.7765e-03	2.03	2.4275e-03	2.02
3.1250e-02	1.4198e-03	2.00	1.9227e-03	2.01	6.0352e-04	2.00
1.5625e-02	3.5497e-04	2.00	4.7951e-04	2.00	1.5066e-04	2.00
7.8125e-03	8.8741e-05	2.00	1.1979e-04	2.00	3.7654e-05	2.00

TABLE 2. Problem case (1): the elliptic reconstruction estimator $\mathcal{E}_N^{\text{ell}}$, the time reconstruction estimators $\mathcal{E}_N^{\text{rec}}(w_n)$, $\mathcal{E}_N^{\text{rec}}(\tilde{w}_n)$ and the corresponding EOCs.

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Time Estimators

$h = k$	$\mathcal{E}_m^{T,1}(w_n)$	EOC	$\mathcal{E}_m^{T,1}(\tilde{w}_n)$	EOC	$\mathcal{E}_m^{T,2}$	EOC	$\mathcal{E}_m^{T,3}$	EOC
1.2500e-01	8.5528e-02		2.6086e-02		1.5603e-01		2.3606e-01	
6.2500e-02	1.9581e-02	2.09	6.0501e-03	2.07	3.9203e-02	1.99	6.0174e-02	1.98
3.1250e-02	4.6603e-03	2.05	1.4486e-03	2.04	9.7796e-03	2.00	1.5116e-02	1.99
1.5625e-02	1.1340e-03	2.02	3.5392e-04	2.02	2.4396e-03	2.00	3.7834e-03	1.99
7.8125e-03	2.7935e-04	2.01	8.7434e-05	2.01	6.0908e-04	2.00	9.4614e-04	2.00

TABLE 3. Problem case (1): the time estimators $\mathcal{E}_N^{T,1}(w_n), \mathcal{E}_N^{T,1}(\tilde{w}_n), \mathcal{E}_N^{T,2}, \mathcal{E}_N^{T,3}$ and the corresponding EOCs.

Space Estimators

$h = k$	$\mathcal{E}_N^{S,1}(w_n)$	EOC	$\mathcal{E}_N^{S,1}(\tilde{w}_n)$	EOC	$\mathcal{E}_N^{S,2}$	EOC
1.2500e-01	3.1258e-02		8.6889e-03		4.0374e-02	
6.2500e-02	4.0411e-03	2.78	1.1079e-03	2.80	1.0095e-02	2.00
3.1250e-02	5.2213e-04	2.78	1.3917e-04	2.82	2.5239e-03	2.00
1.5625e-02	6.7829e-05	2.77	1.7417e-05	2.82	6.3099e-04	2.00
7.8125e-03	8.7779e-06	2.77	2.1778e-06	2.82	1.5775e-04	2.00

TABLE 4. Problem case (1): the space estimators $\mathcal{E}_N^{S,1}(w_n), \mathcal{E}_N^{S,1}(\tilde{w}_n), \mathcal{E}_N^{S,2}$ and the corresponding EOCs.

Errors and Total Estimators

$h = k$	$\max_n \ e^n\ $	EOC	$e_{\text{total}}(t^N)$	EOC	\mathcal{E}_N	$\text{EI}(t^N)$	$\tilde{\mathcal{E}}_N$	$\tilde{\text{EI}}(t^N)$
1.2500e-01	9.7944e-05		2.2317e-03		6.1486e-03	63	1.0842e-02	110
6.2500e-02	2.4658e-05	1.98	1.0163e-03	1.13	1.4988e-03	61	2.7700e-03	112
3.1250e-02	6.1894e-06	1.99	4.8370e-04	1.07	3.6976e-04	60	6.9945e-04	113
1.5625e-02	1.5507e-06	1.99	2.3576e-04	1.03	9.1805e-05	59	1.7569e-04	113
7.8125e-03	3.8811e-07	1.99	1.1636e-04	1.01	2.2905e-05	59	4.4021e-05	113

TABLE 5. Problem case (4): the $L^\infty(0, 1; L^2(\Omega))$ -error, the total error $e_{\text{total}}(t^N)$, and the corresponding EOCs, the two- and three-level estimators \mathcal{E}_N and $\tilde{\mathcal{E}}_N$, respectively, and the corresponding effectivity indices $\text{EI}(t^N)$ and $\tilde{\text{EI}}(t^N)$.

Reconstruction Error Estimators

$h = k$	$\mathcal{E}_{2,N}^{\text{ell}}$	EOC	$\mathcal{E}_{2,N}^{\text{rec}}(w_n)$	EOC	$\mathcal{E}_{2,N}^{\text{rec}}(\tilde{w}_n)$	EOC
1.2500e-01	1.5981e-03		1.3604e-04		1.3604e-04	
6.2500e-02	4.0091e-04	1.99	3.2917e-05	2.04	3.2915e-05	2.04
3.1250e-02	1.0040e-04	1.99	8.1598e-06	2.01	8.1595e-06	2.01
1.5625e-02	2.5122e-05	1.99	2.0353e-06	2.00	2.0353e-06	2.00
7.8125e-03	6.2832e-06	1.99	5.0883e-07	2.00	5.0853e-07	2.00

TABLE 6. Problem case (4): the elliptic reconstruction estimator $\mathcal{E}_N^{\text{ell}}$, the time reconstruction estimators $\mathcal{E}_N^{\text{rec}}(w_n), \mathcal{E}_N^{\text{rec}}(\tilde{w}_n)$ and the corresponding EOCs.

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Time Estimators

$h = k$	$\mathcal{E}_m^{T,1}(w_n)$	EOC	$\mathcal{E}_m^{T,1}(\tilde{w}_n)$	EOC	$\mathcal{E}_m^{T,2}$	EOC	$\mathcal{E}_m^{T,3}$	EOC
1.2500e-01	5.1191e-04		4.7897e-04		2.2811e-03		4.7512e-03	
6.2500e-02	1.1722e-04	2.12	1.1350e-04	2.07	5.6621e-04	2.01	1.2764e-03	1.89
3.1250e-02	2.7942e-05	2.06	2.7502e-05	2.04	1.4086e-04	2.00	3.3022e-04	1.95
1.5625e-02	6.8151e-06	2.03	6.7608e-06	2.02	3.5107e-05	2.00	8.3947e-05	1.97
7.8125e-03	1.6948e-06	2.00	1.6755e-06	2.01	8.7598e-06	2.00	2.1160e-05	1.98

TABLE 7. Problem case (4): the time estimators $\mathcal{E}_N^{T,1}(w_n), \mathcal{E}_N^{T,1}(\tilde{w}_n), \mathcal{E}_N^{T,2}, \mathcal{E}_N^{T,3}$ and the corresponding EOCs.

Space Estimators

$h = k$	$\mathcal{E}_N^{S,1}(w_n)$	EOC	$\mathcal{E}_N^{S,1}(\tilde{w}_n)$	EOC	$\mathcal{E}_N^{S,2}$	EOC
1.2500e-01	1.9954e-04		1.7472e-04		1.4218e-02	
6.2500e-02	2.5050e-05	2.99	2.3489e-05	2.89	3.5650e-02	1.99
3.1250e-02	3.1374e-06	2.99	3.0394e-06	2.95	8.9258e-03	1.99
1.5625e-02	3.9414e-07	2.99	3.8640e-07	2.97	2.2331e-04	1.99
7.8125e-03	7.3976e-08	2.41	4.8704e-08	2.98	5.5849e-04	1.99

TABLE 8. Problem case (4): the space estimators $\mathcal{E}_N^{S,1}(w_n), \mathcal{E}_N^{S,1}(\tilde{w}_n), \mathcal{E}_N^{S,2}$ and the corresponding EOCs.

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