

A POSTERIORI ERROR ESTIMATES FOR THE ALLEN–CAHN PROBLEM*

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Abstract. This work is concerned with the proof of a posteriori error estimates for fully discrete Galerkin approximations of the Allen–Cahn equation in two and three spatial dimensions. The numerical method comprises the backward Euler method combined with conforming finite elements in space. For this method, we prove conditional type a posteriori error estimates in the $L_4(0, T; L_4(\Omega))$ -norm that depend polynomially upon the inverse of the interface length ϵ . The derivation relies crucially on the availability of a spectral estimate for the linearized Allen–Cahn operator about the approximating solution in conjunction with a continuation argument and a variant of the elliptic reconstruction. The new analysis also appears to improve variants of known a posteriori error bounds in $L_2(H^1)$, $L_\infty(L_2)$ -norms in certain regimes.

Key words. Allen–Cahn equation, phase field, discontinuous time-stepping scheme, a posteriori error estimates, conditional estimates

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1. Introduction. The Allen–Cahn problem comprises a singularly perturbed semilinear parabolic partial differential equation (PDE) together with suitable initial and boundary conditions, viz.,

$$(1.1) \quad \begin{aligned} u_t - \Delta u + \frac{1}{\epsilon^2}(u^3 - u) &= f && \text{in } \Omega \times (0, T], \\ u &= 0 && \text{on } \partial\Omega \times (0, T], \\ u(\cdot, 0) &= u_0 && \text{in } \Omega; \end{aligned}$$

we assume that $\Omega \subset \mathbb{R}^d$ is a convex, polygonal ($d = 2$) or polyhedral ($d = 3$) domain of the Euclidean space \mathbb{R}^d , $T \in \mathbb{R}^+$, $0 < \epsilon \ll 1$, for sufficiently smooth initial condition u_0 and forcing function f (precise regularity statements will be given below).

The problem (1.1) belongs to the class of the so-called phase field PDE models for solidification of a pure material, originally introduced by Allen and Cahn [3]

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to describe the phase separation process of a binary alloy at a fixed temperature. The nonlinear function $F(u) := u^3 - u$ is the derivative of the classical *double-well potential* $\int F(u)du$. Due to the nature of the nonlinearity, the solution u develops time-dependent interfaces $\Gamma_t := \{x \in \Omega : u(x, t) = 0\}$, separating regions for which $u \approx 1$ from regions where $u \approx -1$. The solution moves from one region to another within the so-called diffuse interfaces of length $O(\epsilon)$. For a recent comprehensive review of phase field models and their relationship to geometric flows, we refer to [16].

Realistically, ϵ should be orders of magnitude smaller than the physical domain of simulation. Therefore, the accurate and efficient numerical solution of such phase field models requires the resolution of the dynamic diffuse interfaces. This means that the discretization parameters of any numerical method used should provide sufficient numerical resolution to approximate the interface evolution accurately. In the context of finite element methods, this is typically achieved via the use of very fine meshes in the vicinity of the interface region. In an effort to simulate at a tractable computational cost, especially for $d = 3$, it is essential to design adaptive algorithms which are able to dynamically modify the local mesh size.

A standard error analysis of finite element approximations of (1.1) leads to a priori estimates with unfavorable exponential dependence on ϵ^{-1} . This is impractical even for moderately small interface length ϵ . The celebrated works [11, 14, 2] showed that uniform bounds for the principal eigenvalue of the linearized Allen–Cahn spatial operator about the solution u are possible as long as the evolving interface is smooth (cf., (4.8) below). Such spectral estimates are used in the seminal work [18] whereby a priori error bounds with only polynomial dependence on ϵ^{-1} for finite element methods have been proven, enabling also the proof of convergence to the sharp-interface limit. Moreover, assuming the validity of a spectral estimate about the exact solution u , allowed the proof of the first conditional-type a posteriori error bounds for finite element methods approximating the Allen–Cahn problem in the $L_2(H^1)$ -norm, for which the condition depends only polynomially on ϵ ; this was presented in the influential works [23, 17].

This direction of research has taken a further leap forward with the seminal works [5, 7, 8], whereby the principle eigenvalue of the linearized spatial Allen–Cahn operator *about the numerical solution* U_h is used instead, in an effort to arrive to fully computable a posteriori error estimates in the $L_2(H^1)$ - and $L_\infty(L_2)$ -norms, the latter using the elliptic reconstruction framework [25, 24]; see also [19, 9] for application of elliptic reconstruction to nonconforming methods. We also mention [21] whereby a posteriori error bounds in the $L_\infty(L_r)$ -norms, $r \in [2, \infty]$, are proven.

When the interface Γ_t undergoes topological changes, however, e.g., when an interface collapses, unbounded velocities occur and the all-important principal eigenvalue λ can scale like $\lambda \sim \epsilon^{-2}$ on a time interval of length comparable to ϵ^2 . This crucial observation, made in [8], showed that the principal eigenvalue can be assumed to be L_1 -integrable with respect to the time variable allowing, in turn, for robust conditional a posteriori error analysis under topological changes in the $L_2(H^1)$ - and $L_\infty(L_2)$ -norms.

In a recent work [12], a priori bounds for the $L_4(L_4)$ -norm error have been proved, which appear to deliver a rather favorable ϵ^{-1} -polynomial dependence on the respective constant, noting that the $L_4(L_4)$ -norm is present in the stability of the spatial Allen–Cahn operator upon multiplication of (1.1) by u and integration with respect to space and to time. The importance of the $L_4(L_4)$ -norm is evidenced upon interpreting the Allen–Cahn equation as a gradient flow of the energy functional,

$$E(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{4\epsilon^2} (u^2 - 1)^2 \right) dx,$$

related to the *double-well* potential. Then, the Allen–Cahn equation with $f = 0$ arises as the L_2 gradient flow $u_t = -E'(u)$, where $E'(u)$ is understood as the Gâteaux derivative. Upon observing the different scaling with respect to ϵ , it is evident that the quantity $\frac{1}{\epsilon^2} \|u\|_{L_4(\Omega)}^4$ plays a crucial role. An immediate question is whether proving conditional a posteriori error bounds in the $L_4(L_4)$ -norm can also improve the dependence of the condition on the interface length ϵ . Motivated by this, in this work, we prove conditional a posteriori error bounds for the $L_4(L_4)$ -norm for a backward Euler finite element method. The proof is valid under the hypothesis of the existence of a spectral estimate under topological changes in the spirit of [8]. The argument uses a carefully constructed test function, in conjunction with a continuation argument and a new variant of the elliptic reconstruction introduced in [20], as well as known ideas regarding time reconstruction (see [28, 26, 24]). The special test function results in the $\|\cdot\|_{L_4(L_4)}^4$ norm for the quantities requiring estimation. At the same time, the error terms appearing on the right-hand side maintain a typical structure in a posteriori error analysis: they can be separated as time-related and space-related error estimates, data oscillation and mesh-change errors. A key attribute of the new testing is that leading order time- and space-error terms appear inside $\|\cdot\|_{L_2(L_2)}^2$ norms. The discrepancy in powers between the error norm, $\|\cdot\|_{L_4(L_4)}^4$, and the estimator norms, $\|\cdot\|_{L_2(L_2)}^2$, leads to the various ϵ^{-1} -dependent constants in the estimators to have formally milder conditions ensuring the validity of the a posteriori error bounds; cf. also Remark 4.4 below.

As a result of the method of proof, the new a posteriori error analysis provides also new $L_\infty(L_2)$ - and $L_2(H^1)$ -norm a posteriori error bounds which appear to, at least formally, be valid under less stringent smallness conditions compared to results from the literature.

The remainder of this work is structured as follows. The model problem is introduced in section 2. Section 3 includes the definition of the numerical method along with the elliptic and time reconstructions needed for the proof of the main results. The key estimates and the main result are stated and proven in section 4. Section 5 completes the derivation of fully computable error bounds by estimating the terms appearing in the residuals of the main results.

2. Model problem. We denote by $L_p(\Omega)$, $1 \leq p \leq \infty$, the standard Lebesgue spaces with corresponding norms $\|\cdot\|_{L_p(\Omega)}$. Let also $W^{k,p}(\Omega)$ be the k th order of Sobolev space based on $L_p(\Omega)$ and $H^k(\Omega) := W^{k,2}(\Omega)$, $k \geq 0$, along with the corresponding norms $\|\cdot\|_{W^{k,p}(\Omega)}$ and $\|\cdot\|_{H^k(\Omega)}$, respectively. Set $H_0^1(\Omega) := \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$. We shall denote by $\langle \cdot, \cdot \rangle$ the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$, which becomes the standard $L_2(\Omega)$ inner product (\cdot, \cdot) when the arguments are sufficiently smooth. The respective Bochner spaces are denoted by $L_p(0, T; V)$, endowed with the norms

$$\|v\|_{L_p(0,T;V)} = \left(\int_0^T \|v\|_V^p dt \right)^{1/p}, \quad p \in [1, +\infty), \quad \|v\|_{L_\infty(0,T;V)} = \operatorname{ess. sup}_{t \in [0,T]} \|v\|_V$$

with V a Banach space with norm $\|\cdot\|_V$.

We shall make extensive use of the classical *Gagliardo–Nirenberg–Ladyzhenskaya (GNL) inequalities* reading

$$(2.1) \quad \|v\|_{L_4(\Omega)} \leq \tilde{c} \|v\|_{L_2(\Omega)}^{1/2} \|\nabla v\|_{L_2(\Omega)}^{1/2} \quad \text{for } d = 2,$$

$$(2.2) \quad \|v\|_{L_4(\Omega)} \leq \tilde{c} \|v\|_{L_2(\Omega)}^{1/4} \|\nabla v\|_{L_2(\Omega)}^{3/4} \quad \text{for } d = 3$$

for all $v \in H_0^1(\Omega)$ with $\tilde{c} > 0$, independent of v . For later use, we also recall a basic algebraic estimate, often referred to as *Young's inequality*: for any $\delta > 0$, we have

$$ab \leq \delta a^p + C(p, q) \delta^{-\frac{q}{p}} b^q, \quad \text{where } 1/p + 1/q = 1,$$

for any $a, b \geq 0$ and $p, q > 1$, for some $C(p, q) > 0$ independent of a, b .

Let $f \in L_\infty(0, T; L_4(\Omega))$ and $u_0 \in W^{1,4}(\Omega)$. Then, for a.e. $t \in (0, T]$, we seek $u \in L_2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega))$, such that

$$(2.3) \quad \begin{aligned} \langle u_t(t), v \rangle + (\nabla u(t), \nabla v) + \epsilon^{-2} (u^3(t) - u(t), v) &= \langle f(t), v \rangle, \\ (u(0), v) &= (u_0, v), \end{aligned}$$

for all $v \in H_0^1(\Omega)$. Integrating for $t \in (0, T]$, and integrating by parts the above becomes: find $u \in L_2(0, T; H_0^1(\Omega)) \cap L_\infty(0, T; L_2(\Omega))$, such that

$$(2.4) \quad \begin{aligned} (u(T), v(T)) + \int_0^T \left(-\langle u, v_t \rangle + (\nabla u, \nabla v) + \epsilon^{-2} (u^3 - u, v) \right) dt \\ = (u_0, v(0)) + \int_0^T \langle f, v \rangle dt \end{aligned}$$

for all $v \in L_2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega))$.

3. The fully discrete scheme and reconstructions. We shall first present a fully discrete scheme for the Allen–Cahn problem (1.1) by combining the implicit Euler method (lowest order discontinuous Galerkin time-stepping scheme) with conforming finite elements in space. Further, we shall define suitable space and time reconstructions of the fully discrete scheme, which will be crucial for the proof of the a posteriori error bounds below.

3.1. Discretization. Let $0 = t_0 < t_1 < \dots < t_N = T$. We partition the time interval $[0, T]$ into subintervals $J_n := (t_{n-1}, t_n]$ and we denote by $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ each time step.

Let also $\{\mathcal{T}_h^n\}_{n=0}^N$ be a sequence of conforming and shape-regular triangulations of the domain Ω , that are allowed to be modified between time steps. We define the mesh size function, $h_n : \Omega \rightarrow \mathbb{R}$, by $h_n(x) := \text{diam}(\tau)$, $x \in \tau$ for $\tau \in \mathcal{T}_h^n$. With each \mathcal{T}_h^n we associate the finite element space

$$V_h^n := \{\chi \in C(\bar{\Omega}); \chi|_\tau \in \mathbb{P}_\kappa(\tau) \ \forall \tau \in \mathcal{T}_h^n\}$$

with \mathbb{P}_κ denoting the d -variate space of polynomials of degree at most $\kappa \in \mathbb{N}$. The whole theory presented below remains valid if box-type elements are used and respective polynomial spaces of degree κ on each variable.

We say that a set of triangulations is *compatible* when they are constructed by different refinements of the same (coarser) triangulation. Given two compatible triangulations \mathcal{T}_h^{n-1} and \mathcal{T}_h^n , we consider their *finest common coarsening* $\hat{\mathcal{T}}_h^n := \mathcal{T}_h^n \wedge \mathcal{T}_h^{n-1}$ and set $\hat{h}_n := \max(h_n, h_{n-1})$. Furthermore, we denote by \mathcal{S}_h^n the interior mesh skeleton of \mathcal{T}_h^n , and we define the sets $\hat{\mathcal{S}}_h^n := \mathcal{S}_h^n \cap \mathcal{S}_h^{n-1}$ and $\check{\mathcal{S}}_h^n := \mathcal{S}_h^n \cup \mathcal{S}_h^{n-1}$. We note that no assumption on the relative size of \hat{h}_n compared to the sizes h_{n-1}, h_n is necessary for the validity of the estimates presented below. Reconstruction-based a posteriori error analysis for parabolic problems is also possible under the extreme mesh-modification scenario of no strict finest common coarsening subspace, i.e., when $\hat{\mathcal{T}}_h^n = \{\Omega\}$; we refer to [10] for a detailed discussion. We do not envisage an insurmountable technical obstacle in extending the present analysis to such an extreme scenario.

Approximations will be subordinate to the time partition. A finite element space $V_h^n \subset H_0^1(\Omega)$ is specified on each time interval J_n , $n = 1, \dots, N$. Then, we seek approximate solutions from the space

$$V_{hk} := \{X \in L_2(0, T; H_0^1(\Omega)); X|_{J_n} \in \mathbb{P}_0[J_n : V_h^n], n = 1, \dots, N\}$$

with $\mathbb{P}_0[J_n; V_h^n]$ denoting the space of constant polynomials over J_n , having values in V_h^n ; these functions are allowed to be discontinuous at the nodal points, but are taken to be continuous from the left.

3.2. Fully discrete scheme. For brevity, we set $F(v) := v^3 - v$. The backward Euler finite element method reads, for each $n = 1, \dots, N$, find $U_h^n \in V_h^n$ such that

$$(3.1) \quad k_n^{-1} (U_h^n - U_h^{n-1}, X) + (\nabla U_h^n, \nabla X) + \epsilon^{-2} (F(U_h^n), X) = \langle f^n, X \rangle, \\ U_h^0 = \mathcal{P}_h^0 u^0,$$

for every $X \in V_{hk}$ with $f^n := f(t_n)$ and \mathcal{P}_h^n denoting the orthogonal L_2 -projection operator onto V_h^n .

Let now $\Delta_h^n : V_h^n \rightarrow V_h^n$ defined by $(-\Delta_h^n V, X) = (\nabla V, \nabla X)$ for all $V, X \in V_h^n$, i.e., the discrete Laplacian. This allows for the strong representation of (3.1) as

$$(3.2) \quad k_n^{-1} (U_h^n - \mathcal{P}_h^n U_h^{n-1}) - \Delta_h^n U_h^n + \epsilon^{-2} \mathcal{P}_h^n F(U_h^n) = \mathcal{P}_h^n f^n.$$

We now introduce a variant of the elliptic reconstruction [25, 24, 20], which will be instrumental in the proof of the a posteriori error bounds below.

DEFINITION 3.1 (elliptic reconstruction). *For each $n = 0, 1, \dots, N$, we define the elliptic reconstruction $\omega^n \in H_0^1(\Omega)$ to be the solution of the elliptic problem*

$$(3.3) \quad (\nabla \omega^n, \nabla v) = \langle g_h^n, v \rangle \quad \text{for all } v \in H_0^1(\Omega),$$

where

$$(3.4) \quad g_h^n := -\Delta_h^n U_h^n - \epsilon^{-2} (F(U_h^n) - \mathcal{P}_h^n F(U_h^n)) - \mathcal{P}_h^n f^n + f^n \\ - k_n^{-1} (\mathcal{P}_h^n U_h^{n-1} - U_h^{n-1});$$

here and in the following we adopt the convention $U_h^{-1} := U_h^0$.

Remark 3.2 (Galerkin orthogonality). We observe that ω^n satisfies

$$(3.5) \quad (\nabla(\omega^n - U_h^n), \nabla X) = 0 \quad \text{for all } X \in V_h^n.$$

This relation implies that $\omega^n - U_h^n$ is orthogonal to V_h^n with respect to the Dirichlet inner product, a crucial property that allows us to use a posteriori error bounds for elliptic problems to estimate various norms of $\omega^n - U_h^n$ from above; we refer to section 5 for a detailed discussion.

DEFINITION 3.3 (time reconstruction). *For $t \in J_n$, $n = 1, \dots, N$, we set*

$$(3.6) \quad U_h(t) := \ell_{n-1}(t)U_h^{n-1} + \ell_n(t)U_h^n \quad \text{and} \quad \omega(t) := \ell_{n-1}(t)\omega^{n-1} + \ell_n(t)\omega^n,$$

where ℓ_n is the piecewise linear Lagrange basis function with $\ell_n(t_k) = \delta_{kn}$.

Notice that U_h , w are continuous functions with respect to time. The above definition implies that the time derivative of U_h ,

$$(3.7) \quad U_{h,t}(t) = \frac{U_h^n - U_h^{n-1}}{k_n},$$

is the discrete backward difference at t_n .

4. A posteriori error estimates. We shall now use the reconstructions defined above, together with nonstandard energy and continuation arguments and a spectral estimate for the linearized steady-state problem about the approximate solution U_h , to arrive at a posteriori error bounds in the $L_4(L_4)$ -, $L_2(H^1)$ -, and $L_\infty(L_2)$ -norms.

4.1. Error relation. We begin by splitting the total error as follows:

$$(4.1) \quad e := u - U_h = \theta - \rho, \quad \text{where} \quad \theta := \omega - U_h, \quad \rho := \omega - u.$$

In view of Remark 3.2, θ can be estimated by a posteriori error bounds for elliptic problems in various norms.

Also, ρ satisfies an equation of the form (2.3) with a fully computable right-hand side that consists of θ and the problem data. To see this, (2.3) along with Definitions 3.1 and 3.3 and elementary manipulations lead to the following result.

LEMMA 4.1 (error equation). *On J_n , $n = 1, \dots, N$, and for all $v \in H_0^1(\Omega)$, we have*

$$(4.2) \quad \begin{aligned} & \langle \rho_t, v \rangle + (\nabla \rho, \nabla v) + \epsilon^{-2} (F(U_h) - F(u), v) \\ &= \langle f^n - f, v \rangle + \langle \theta_t, v \rangle + \epsilon^{-2} (F(U_h) - F(U_h^n), v) + (\nabla(\omega - \omega^n), \nabla v). \end{aligned}$$

Therefore, norms of ρ can be estimated through PDE stability arguments; this will be performed below. Before doing so, however, we further estimate the term involving the elliptic reconstructions on the right-hand side from (4.2). For brevity, we set $\partial X_n := (X_n - X_{n-1})/k_n$ for any sequence $\{X_n\}_{n \in \mathbb{N} \cup \{0\}}$.

LEMMA 4.2. *On J_n , $n = 1, \dots, N$, we have*

$$(4.3) \quad \begin{aligned} (\nabla(\omega - \omega^n), \nabla v) &\leq \left(\|\partial U_h^n - \partial U_h^{n-1}\|_{L_2(\Omega)} + \epsilon^{-2} \|F(U_h^n) - F(U_h^{n-1})\|_{L_2(\Omega)} \right. \\ &\quad \left. + \|f^n - f^{n-1}\|_{L_2(\Omega)} \right) \|v\|_{L_2(\Omega)} \end{aligned}$$

for all $v \in H_0^1(\Omega)$.

Proof. From (3.6) and Definition 3.1, we can write

$$\begin{aligned} (\nabla(\omega - \omega^n), \nabla v) &= \ell_{n-1}(t) (\nabla(\omega^{n-1} - \omega^n), \nabla v) \\ &= \ell_{n-1}(t) (g_h^{n-1} - g_h^n, v) \leq \|g_h^{n-1} - g_h^n\|_{L_2(\Omega)} \|v\|_{L_2(\Omega)}. \end{aligned}$$

Then, using (3.4) in conjunction with (3.2), we obtain

$$\begin{aligned} g_h^n &= -k_n^{-1} (U_h^n - \mathcal{P}_h^n U_h^{n-1}) - \epsilon^{-2} F(U_h^n) + f^n - k_n^{-1} (\mathcal{P}_h^n U_h^{n-1} - U_h^{n-1}) \\ &= k_n^{-1} (U_h^{n-1} - U_h^n) - \epsilon^{-2} F(U_h^n) + f^n, \end{aligned}$$

and correspondingly for g_h^{n-1} . Combining the above, the result already follows. \square

4.2. Energy argument. We begin by introducing some notation. We define

$$\begin{aligned} \mathcal{L}_1 &:= \|\partial U_h^n - \partial U_h^{n-1}\|_{L_2(\Omega)}^2 + \epsilon^{-4} \|F(U_h^n) - F(U_h^{n-1})\|_{L_2(\Omega)}^2 + \|f^n - f^{n-1}\|_{L_2(\Omega)}^2, \\ \mathcal{L}_2 &:= \|f^n - f\|_{L_2(\Omega)}^2 + \epsilon^{-4} \|F(U_h^n) - F(U_h^n)\|_{L_2(\Omega)}^2, \end{aligned}$$

on each J_n , $n = 1, \dots, N$, noting that $\mathcal{L}_2 \equiv \mathcal{L}_2(t)$; for $n = 1$ we adopt the convention that $U_h^{-1} = U_h^0$.

Moreover, for brevity, we also set

$$\begin{aligned}\Theta_1 &\equiv \Theta_1(t) := \frac{1}{2}\|\theta_t\|_{L_2(\Omega)}^2 + \frac{11}{4}C_{PF}^4\|\theta_t\|_{L_4(\Omega)}^4, \\ \Theta_2 &\equiv \Theta_2(t) := \epsilon^{-4}\left((C_0 + 396\|U_h\|_{L_\infty(\Omega)}^2)\|\theta\|_{L_2(\Omega)}^2 + \frac{C_1}{2}\|\theta\|_{L_4(\Omega)}^4 + C_0\|\theta\|_{L_6(\Omega)}^6\right), \\ A(t) &:= \epsilon^{-2}\left(\left(\theta^2\rho^2 + \rho^4 + |\nabla\rho|^2, \int_t^\tau \rho^2(s) \, ds\right) + (\theta^2, \rho^2)\right),\end{aligned}$$

where $C_0 := (C_{PF}\tilde{c}^2 + 1)/2$, $C_1 := 9 + 9C_{PF}\tilde{c}^2 + 6^4 11^2 C_{PF}^2 \tilde{c}^4$, $C_2 := 2 \cdot 3^7 C_{PF}^2 \tilde{c}^4$, where C_{PF} is the constant of the Poincaré–Friedrichs inequality $\|v\| \leq C_{PF}\|\nabla v\|$ and \tilde{c} as in (2.1).

LEMMA 4.3 ($d = 2$). *Let $d = 2$ and u be the solution of (2.3) and ω as in (3.6). Assume that $\rho(t) \in W_0^{1,4}(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, we have*

$$\begin{aligned}(4.4) \quad & \frac{1}{4} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 \, dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ & + \int_0^\tau A(t) \, dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h)\rho, \rho) \right) dt \\ & \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_{PF}^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \Theta_2 + C_0(\mathcal{L}_1 + \mathcal{L}_2)) \, dt \\ & + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2 + \alpha(U_h) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & + \frac{1}{4\epsilon^6} \int_0^\tau \left(\beta(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4 + \gamma(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt,\end{aligned}$$

where

$$\begin{aligned}\alpha(U_h) &:= \|F'(U_h)\|_{L_\infty(\Omega)}^2 + \|U_h\|_{L_\infty(\Omega)}^2 + 7 \\ \beta(\theta, U_h) &:= \frac{C_2\epsilon^4}{16} (\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4) + 2\epsilon^2 \|U_h\|_{L_\infty(\Omega)}^4 \\ &\quad + 2C_{PF}^2 \tilde{c}^4 \|F'(U_h)\|_{L_\infty(\Omega)}^2 + 11\epsilon^6 (\|F'(U_h)\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4 + 6), \\ \gamma(\theta, U_h) &:= 2\tilde{c}^4 \left(C_{PF}^2 \|F'(U_h)\|_{L_\infty(\Omega)}^2 + 36 (\|\theta\|_{L_\infty(\Omega)}^2 + \|U_h\|_{L_\infty(\Omega)}^2) \right).\end{aligned}$$

Proof. Using Taylor's theorem, we immediately deduce

$$F(U_h) - F(u) = -eF'(U_h) - 3e^2U_h - e^3.$$

Let $\phi : [0, \tau] \times \Omega \rightarrow \mathbb{R}$ for $0 < \tau \leq T$, such that

$$(4.5) \quad \phi(\cdot, t) = \rho(\cdot, t) \left(\int_t^\tau \rho^2(\cdot, s) \, ds + 1 \right), \quad t \in [0, \tau].$$

The hypothesis $\rho \in W_0^{1,4}(\Omega)$ implies that $\phi \in H_0^1(\Omega)$. Setting $v = \phi$ in (4.2), we have

$$\begin{aligned}\langle \rho_t, \phi \rangle + (\nabla \rho, \nabla \phi) - \epsilon^{-2} (eF'(U_h) + 3e^2U_h + e^3, \phi) &= \langle f^n - f, \phi \rangle + \langle \theta_t, \phi \rangle \\ &\quad + \epsilon^{-2} (F(U_h) - F(U_h^n), \phi) + (\nabla(\omega - \omega^n), \nabla \phi).\end{aligned}$$

Observing now the identities

$$\begin{aligned}(e^2 U_h, \phi) &= (\theta^2 U_h, \phi) + (\rho^2 U_h, \phi) - 2(\theta \rho U_h, \phi), \\ (e^3, \phi) &= (\theta^3, \phi) - 3(\theta^2 \rho, \phi) + 3(\theta \rho^2, \phi) - (\rho^3, \phi),\end{aligned}$$

elementary calculations yield

$$\begin{aligned}(4.6) \quad & \frac{1}{2} \frac{d}{dt} \|\rho\|_{L_2(\Omega)}^2 + \left\langle \rho_t, \rho \int_t^\tau \rho^2(s) ds \right\rangle + \left(\nabla \rho, \rho \int_t^\tau \nabla \rho^2(s) ds \right) \\ & + \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h) \rho, \rho) + \epsilon^{-2} \|\rho\|_{L_4(\Omega)}^4 + A(t) \\ & = \langle f^n - f, \phi \rangle + \langle \theta_t, \phi \rangle + \epsilon^{-2} (F(U_h) - F(U_h^n), \phi) + (\nabla(\omega - \omega^n), \nabla \phi) \\ & + 3\epsilon^{-2} (\theta^2 U_h, \phi) + 3\epsilon^{-2} (\rho^2 U_h, \phi) - 6\epsilon^{-2} (\theta \rho U_h, \phi) + \epsilon^{-2} (\theta^3, \phi) \\ & + 3\epsilon^{-2} (\theta \rho^2, \phi) + \epsilon^{-2} (F'(U_h) \theta, \phi) - \epsilon^{-2} \left(F'(U_h) \rho, \rho \int_t^\tau \rho^2(s) ds \right) =: \sum_{j=1}^{11} I_j.\end{aligned}$$

We shall further estimate each I_j . We begin by splitting I_1 into

$$I_1 = \left\langle f^n - f, \rho \int_t^\tau \rho^2(s) ds \right\rangle + \langle f^n - f, \rho \rangle =: I_1^1 + I_1^2.$$

Applying the Hölder, GNL for $d = 2$, Poincaré–Friedrichs and Young inequalities gives, respectively,

$$\begin{aligned}I_1^1 &\leq \|f^n - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq \tilde{c} \|f^n - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \\ &\leq C_{PF}^{1/2} \tilde{c} \|f^n - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{C_{PF} \tilde{c}^2}{2} \|f^n - f\|_{L_2(\Omega)}^2 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{11}{4} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4.\end{aligned}$$

The Cauchy–Schwarz and Young inequalities also yield $I_1^2 \leq \frac{1}{2} \mathcal{L}_2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2$. Likewise, we split I_3 as follows:

$$I_3 = \epsilon^{-2} (F(U_h) - F(U_h^n), \rho \int_t^\tau \rho^2(s) ds) + \epsilon^{-2} (F(U_h) - F(U_h^n), \rho) =: I_3^1 + I_3^2,$$

yielding the following bounds:

$$\begin{aligned}I_3^1 &\leq \frac{C_{PF} \tilde{c}^2}{2\epsilon^4} \|F(U_h) - F(U_h^n)\|_{L_2(\Omega)}^2 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{11}{4} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_3^2 &\leq \frac{1}{2\epsilon^4} \|F(U_h) - F(U_h^n)\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2.\end{aligned}$$

From Lemma 4.2 and working as before, we have

$$I_4 = \left(\nabla(\omega - \omega^n), \nabla \left(\rho \int_t^\tau \rho^2(s) \, ds \right) \right) + (\nabla(\omega - \omega^n), \nabla \rho) := I_4^1 + I_4^2,$$

$$I_4^1 \leq \frac{C_{PF}\tilde{c}^2}{2} \mathcal{L}_1 + \frac{3}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{33}{4} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4,$$

$$I_4^2 \leq \frac{1}{2} \mathcal{L}_1 + \frac{3}{2} \|\rho\|_{L_2(\Omega)}^2.$$

Next, we split I_2 as follows:

$$I_2 = \left\langle \theta_t, \rho \int_t^\tau \rho^2(s) \, ds \right\rangle + \langle \theta_t, \rho \rangle =: I_2^1 + I_2^2$$

and, using the Hölder, Poincaré–Friedrichs, and Young inequalities, we deduce

$$\begin{aligned} I_2^1 &\leq \|\theta_t\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq C_{PF} \|\theta_t\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{11C_{PF}^4}{4} \|\theta_t\|_{L_4(\Omega)}^4 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{1}{2} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2, \\ I_2^2 &\leq \frac{1}{2} \|\theta_t\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

Next, we split

$$I_5 = 3\epsilon^{-2} \left(\theta^2 U_h, \rho \int_t^\tau \rho^2(s) \, ds \right) + 3\epsilon^{-2} (\theta^2 U_h, \rho) =: I_5^1 + I_5^2,$$

which can be further bounded as follows:

$$\begin{aligned} I_5^1 &\leq 3\epsilon^{-2} \|\theta^2\|_{L_2(\Omega)} \|U_h\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\ &\leq 3\epsilon^{-2} \tilde{c} \|\theta\|_{L_4(\Omega)}^2 \|U_h\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)}^{1/2} \left\| \nabla \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)}^{1/2} \\ &\leq 3\epsilon^{-2} C_{PF}^{1/2} \tilde{c} \|\theta\|_{L_4(\Omega)}^2 \|U_h\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{9C_{PF}\tilde{c}^2}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{11}{4} \|U_h\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\ I_5^2 &\leq \frac{9}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{2} \|U_h\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

In the same spirit, we also have

$$I_7 = -6\epsilon^{-2} \left(\theta \rho U_h, \rho \int_t^\tau \rho^2(s) \, ds \right) - 6\epsilon^{-2} (\theta \rho U_h, \rho) =: I_7^1 + I_7^2$$

and, thus,

$$\begin{aligned}
 I_7^1 &\leq 6\epsilon^{-2} \|\theta\|_{L_4(\Omega)} \|\rho^2\|_{L_2(\Omega)} \|U_h\|_{L_\infty(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\
 &\leq \frac{6C_{PF}^{1/2} \tilde{C}}{\epsilon^2} \|\theta\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \|U_h\|_{L_\infty(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \frac{6^4 11^2 C_{PF}^2 \tilde{C}^4}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{1}{2\epsilon^4} \|U_h\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\
 I_7^2 &\leq \frac{6}{\epsilon^2} \|\theta\|_{L_2(\Omega)} \|U_h\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \leq \frac{396}{\epsilon^4} \|U_h\|_{L_\infty(\Omega)}^2 \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4.
 \end{aligned}$$

Next, we consider the splitting

$$I_{10} = \epsilon^{-2} (F'(U_h)\theta, \rho \int_t^\tau \rho^2(s) \, ds) + \epsilon^{-2} (F'(U_h)\theta, \rho) =: I_{10}^1 + I_{10}^2,$$

and we have the following bounds:

$$\begin{aligned}
 I_{10}^1 &\leq \epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\theta\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\
 &\leq \frac{C_{PF}^{1/2} \tilde{C}}{\epsilon^2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\theta\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \frac{C_{PF} \tilde{C}^2}{2\epsilon^4} \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{11}{4} \|F'(U_h)\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\
 I_{10}^2 &\leq \frac{1}{2\epsilon^4} \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{2} \|F'(U_h)\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^2.
 \end{aligned}$$

Next, we set

$$I_8 = \epsilon^{-2} \left(\theta^3, \rho \int_t^\tau \rho^2(s) \, ds \right) + \epsilon^{-2} (\theta^3, \rho) =: I_8^1 + I_8^2,$$

and we further estimate as follows:

$$\begin{aligned}
 I_8^1 &\leq \epsilon^{-2} \|\theta^3\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\
 &\leq \frac{C_{PF}^{1/2} \tilde{C}}{\epsilon^2} \|\theta\|_{L_6(\Omega)}^3 \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \frac{C_{PF} \tilde{C}^2}{2\epsilon^4} \|\theta\|_{L_6(\Omega)}^6 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4 + \frac{11}{4} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\
 I_8^2 &\leq \frac{1}{2\epsilon^4} \|\theta\|_{L_6(\Omega)}^6 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2.
 \end{aligned}$$

For I_6 and I_9 , we work collectively as follows:

$$I_6 + I_9 = 3\epsilon^{-2} \left(\rho^2(U_h + \theta), \rho \int_t^\tau \rho^2(s) \, ds \right) + 3\epsilon^{-2} (\rho^2(U_h + \theta), \rho) =: I_{6,9}^1 + I_{6,9}^2,$$

and estimate

$$\begin{aligned}
 I_{6,9}^1 &\leq \frac{3C_{PF}^{1/2}\tilde{c}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \left(\|\theta\|_{L_\infty(\Omega)} + \|U_h\|_{L_\infty(\Omega)} \right) \left\| \nabla \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \epsilon^{-2} \|\rho\|_{L_4(\Omega)}^4 + \frac{C_2}{64\epsilon^2} \left(\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4 \right) \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\
 I_{6,9}^2 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^2 \left(\|\theta\|_{L_\infty(\Omega)} + \|U_h\|_{L_\infty(\Omega)} \right) \|\rho\|_{L_2(\Omega)} \\
 &\leq \frac{3\tilde{c}^2}{\epsilon^2} \|\nabla \rho\|_{L_2(\Omega)} \left(\|\theta\|_{L_\infty(\Omega)} + \|U_h\|_{L_\infty(\Omega)} \right) \|\rho\|_{L_2(\Omega)}^2 \\
 &\leq \frac{\epsilon^2}{4} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{18\tilde{c}^4}{\epsilon^6} \left(\|\theta\|_{L_\infty(\Omega)}^2 + \|U_h\|_{L_\infty(\Omega)}^2 \right) \|\rho\|_{L_2(\Omega)}^4.
 \end{aligned}$$

Finally for the last term on the right-hand side of (4.6), we have

$$\begin{aligned}
 I_{11} &\leq \epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \frac{C_{PF}\tilde{c}^2}{\epsilon^2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \|\nabla \rho\|_{L_2(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\
 &\leq \frac{\epsilon^2}{4} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{C_{PF}^2\tilde{c}^4}{2\epsilon^6} \|F'(U_h)\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^4 \\
 &\quad + \frac{C_{PF}^2\tilde{c}^4}{2\epsilon^6} \|F'(U_h)\|_{L_\infty(\Omega)}^2 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4.
 \end{aligned}$$

Applying the above estimates into (4.6) and integrating with respect to $t \in (0, \tau)$ and observing the identities,

$$\begin{aligned}
 \int_0^\tau \left\langle \rho_t, \rho \int_t^\tau \rho^2(s) \, ds \right\rangle dt &= -\frac{1}{2} \left\langle \rho^2(0), \int_0^\tau \rho^2(s) \, ds \right\rangle + \frac{1}{2} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 \, dt, \\
 \int_0^\tau \left(\nabla \rho, \rho \int_t^\tau \nabla \rho^2(s) \, ds \right) dt &= -\frac{1}{4} \int_0^\tau \frac{d}{dt} \left(\int_t^\tau \nabla \rho^2(s) \, ds, \int_t^\tau \nabla \rho^2(s) \, ds \right) dt \\
 &= \frac{1}{4} \left\| \int_0^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2;
 \end{aligned}$$

along with elementary manipulations, the result already follows. \square

The terms in \mathcal{L}_1 and the term $\epsilon^{-4} \|F(U_h) - F(U_h^n)\|_{L_2(\Omega)}^2$ of \mathcal{L}_2 are often referred to as the *time error estimates* in the a posteriori error estimation literature for evolution problems. Correspondingly, $\|f^n - f\|_{L_2(\Omega)}^2$ is the *data approximation*. Θ_1 represents the *mesh change* and Θ_2 (or $\tilde{\Theta}_2$, respectively) is often termed the *spatial error estimate*. These will be presented in detail in section 5.

Remark 4.4. A key ingredient in the proof above is the nonstandard test function ϕ given in (4.5). This test function is responsible for the appearance of the term $\|\rho\|_{L_4(0,T;L_4(\Omega))}^4$, together with other *nonnegative* terms on the left-hand side of (4.4) in the course of the energy argument. At the same time, this test function is also re-

sponsible for the presence of favorable computable error terms in the $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$ norm; cf., for instance, the terms in $\int_0^\tau (\mathcal{L}_1 + \mathcal{L}_2) dt$ that will eventually appear in the final estimate. Thus, the dependence on ϵ of the constants multiplying various terms in \mathcal{L}_1 and \mathcal{L}_2 will be halved due to the discrepancy between the fourth power appearing in the error terms and the second power in the respective estimators. This observation leads to a formally better dependence with respect to ϵ^{-1} in the continuation argument. At the same time, the choice (4.5) results in terms involving $\|\theta\|_{L_4(0,T;L_4(\Omega))}^4$, $\|\theta\|_{L_6(0,T;L_6(\Omega))}^6$, and $\|\theta_t\|_{L_4(0,T;L_4(\Omega))}^4$ without any detriment to the formal dependence on ϵ^{-1} either, as we shall see in the discussion below. The latter terms are “compatible” with the norms of the error ρ appearing in (4.4).

The use of the dimension-dependent GNL inequalities (2.1)–(2.2) necessitates certain modifications in the above argument when $d = 3$, which we now provide. For brevity, we shall only provide the terms which are handled differently from the proof of the two-dimensional case from Lemma 4.3. Nonetheless, the advantages described in Remark 4.4 persist for the three-dimensional case.

LEMMA 4.5 ($d = 3$). *Let $d = 3$, u the solution of (2.3), and ω as in (3.6). Assume that $\rho(t) \in W_0^{1,4}(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, we have*

$$\begin{aligned}
 & \frac{1}{8} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\
 & + \int_0^\tau A(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h)\rho, \rho) \right) dt \\
 (4.7) \quad & \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_{PF}^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \tilde{\Theta}_2 + \tilde{C}_0(\mathcal{L}_1 + \mathcal{L}_2)) dt \\
 & + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + (\alpha(U_h) + 1) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\
 & + \frac{1}{4\epsilon^{10}} \int_0^\tau \left(\tilde{\beta}(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \tilde{\gamma}(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt,
 \end{aligned}$$

where

$$\begin{aligned}
 \tilde{\Theta}_2 &:= \epsilon^{-4} \left((\tilde{C}_0 + 396 \|U_h\|_{L_\infty(\Omega)}^2) \|\theta\|_{L_2(\Omega)}^2 + \frac{\tilde{C}_1}{2} \|\theta\|_{L_4(\Omega)}^4 + \tilde{C}_0 \|\theta\|_{L_6(\Omega)}^6 \right), \\
 \tilde{\beta}(\theta, U_h) &:= \frac{\tilde{C}_2 \epsilon^8}{16} (\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4) + 2\epsilon^6 \|U_h\|_{L_\infty(\Omega)}^4 \\
 &\quad + 2C_{PF} \tilde{c}^4 \epsilon^2 \|F'(U_h)\|_{L_\infty(\Omega)}^4 + 11\epsilon^{10} (\|F'(U_h)\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4 + 6), \\
 \tilde{\gamma}(\theta, U_h) &:= 324C_{PF} \tilde{c}^4 (\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4)
 \end{aligned}$$

with $\tilde{C}_0 := (C_{PF}^{1/2} \tilde{c}^2 + 1)/2$, $\tilde{C}_1 := 9 + 9C_{PF}^{1/2} \tilde{c}^2 + 6^4 11^2 C_{PF} \tilde{c}^4$, $\tilde{C}_2 := 3^7 C_{PF} \tilde{c}^4$.

Proof. Starting from (4.6), we discuss only the different treatment of the terms I_j , $j = 6, 9, 11$; the estimation of the remaining terms is identical to the proof of Lemma 4.3 and is, therefore, omitted. To that end, we begin by setting $\zeta(\theta, U_h) :=$

$\|\theta\|_{L_\infty(\Omega)} + \|U_h\|_{L_\infty(\Omega)}$. Then, we have

$$\begin{aligned} I_{6,9}^1 &\leq \frac{3}{\epsilon^2} \|\rho^3\|_{L_{4/3}(\Omega)} \zeta(\theta, U_h) \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\ &\leq \frac{3\tilde{C}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \zeta(\theta, U_h) \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)}^{1/4} \left\| \nabla \int_t^\tau \rho^2(s) \, ds \right\|_{L_2(\Omega)}^{3/4} \\ &\leq \frac{3\tilde{C}C_{PF}^{1/4}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \zeta(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{2\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{\tilde{C}_2}{64\epsilon^2} \left(\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4 \right) \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \end{aligned}$$

using (2.1) for $d = 3$. Similarly, we have

$$\begin{aligned} I_{6,9}^2 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^2 \zeta(\theta, U_h) \|\rho\|_{L_2(\Omega)} \leq \frac{3\tilde{C}}{\epsilon^2} \|\rho\|_{L_2(\Omega)}^{1/4} \|\nabla \rho\|_{L_2(\Omega)}^{3/4} \|\rho\|_{L_4(\Omega)} \zeta(\theta, U_h) \|\rho\|_{L_2(\Omega)} \\ &\leq \frac{3C_{PF}^{1/4}\tilde{C}}{\epsilon^2} \|\nabla \rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \zeta(\theta, U_h) \|\rho\|_{L_2(\Omega)} \\ &\leq \frac{\epsilon^2}{2} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{18C_{PF}^{1/2}\tilde{C}^2}{\epsilon^6} \|\rho\|_{L_4(\Omega)}^2 \left(\|\theta\|_{L_\infty(\Omega)}^2 + \|U_h\|_{L_\infty(\Omega)}^2 \right) \|\rho\|_{L_2(\Omega)}^2 \\ &\leq \frac{\epsilon^2}{2} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{81C_{PF}\tilde{C}^4}{\epsilon^{10}} \left(\|\theta\|_{L_\infty(\Omega)}^4 + \|U_h\|_{L_\infty(\Omega)}^4 \right) \|\rho\|_{L_2(\Omega)}^4. \end{aligned}$$

Likewise, using completely analogous arguments, we have

$$\begin{aligned} I_{11} &\leq \epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\ &\leq \frac{C_{PF}^{1/4}\tilde{C}}{\epsilon^2} \|F'(U_h)\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 + \frac{1}{8} \|\rho\|_{L_4(\Omega)}^4 + \frac{C_{PF}\tilde{C}^4}{2\epsilon^8} \|F'(U_h)\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4. \end{aligned}$$

The estimation of the remaining I_j on the right-hand side of (4.6) is completely analogous to the two-dimensional case with the difference that one applies (2.1) for $d = 3$. Collecting all the estimates, we arrive at the desirable result. \square

Remark 4.6. We stress that the above result remains valid for the case of Neumann boundary conditions upon modifying slightly the definition of the elliptic reconstruction (3.3) to eliminate the undetermined mode. Moreover, this can be done in such a way to recover (2.1) for terms involving ρ . This is not done here in the interest of simplicity of the presentation only.

4.3. Spectral estimates. To ensure polynomial dependence of the resulting estimates on ϵ^{-1} , a widely used idea is to employ *spectral estimates* of the principal eigenvalue of the linearized Allen–Cahn operator:

$$(4.8) \quad -\lambda(t) := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\|\nabla v\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(u)v, v)}{\|v\|_{L_2(\Omega)}^2}.$$

The celebrated works [11, 14, 2] showed that λ can be bounded independently of ϵ for the case of smooth, evolved interfaces. This idea was used in the seminal works [18] for

the proof of a priori and [23, 17] for a posteriori error bounds for finite element methods in various norms with constants depending upon ϵ^{-1} only in a polynomial fashion. The a priori nature of the spectral estimate (4.8) is somewhat at odds, however, with the presence of λ in a posteriori error bounds. This difficulty was overcome in the seminal work [5] by first linearizing about the numerical solution U_h , viz.,

$$(4.9) \quad -\lambda_h(t) := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\|\nabla v\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h)v, v)}{\|v\|_{L_2(\Omega)}^2},$$

and by then proving verifiable eigenvalue approximation error bounds. The latter ensures that it is possible to compute principle eigenvalue approximations, such that $\Lambda_h \geq \lambda_h$; we refer to [5, section 5] for the detailed construction. In short, it has been shown that for linear conforming finite element spaces, ($\kappa = 1$), it is possible to construct $\Lambda_h(t) \geq \lambda_h(t)$ for almost all $t \in (0, T]$ upon assuming that $\|U_h\|_{L_\infty(\Omega)}$ remains bounded independently of ϵ^{-1} .

The ϵ -independence λ (resp., λ_h , Λ_h), however, is *not* guaranteed when the evolving interfaces are subjected to topological changes. This is an important challenge, since phase-field approaches are preferred over sharp-interface models exactly due to their ability to evolve interfaces past topological changes. To address this, in [8] (cf., also [6, 7]) a crucial observation on the temporal integrability of λ under topological changes was given: during topological changes we have $\lambda(t) \sim \epsilon^{-2}$, but *only* for time periods of length ϵ^2 . Therefore, it has been postulated that there exists an $m > 0$ such that

$$(4.10) \quad \int_0^T (\lambda(t))_+ dt \leq C + \log(\epsilon^{-m})$$

holds for some constant $C > 0$ independent of ϵ , here $\nu_+ := \max\{\nu, 0\}$; notice that for $m = 0$, we return to the earlier case of no topological changes. A number of numerically validated scenarios justifying (4.10) for the scalar Allen–Cahn and its vectorial counterpart, the Ginzburg–Landau equation, can be found in [8]. Moreover, a construction for a $\Lambda_h \in L_1(0, T)$ such that

$$(4.11) \quad \int_0^T (\Lambda_h(t))_+ dt \geq \int_0^T (\lambda_h(t))_+ dt,$$

has been provided in [8, Proposition 3.8].

The above motivate the following assumption on the behavior of the principal eigenvalue λ_h , which we shall henceforth adopt.

Assumption 4.7. We postulate the validity of one of the following options:

- (I) We assume that the zero level set $\Gamma_t = \{x \in \Omega : u(x, t) = 0\}$ is sufficiently smooth. Then, for almost every $t \in (0, T]$, there exists a computable bound $\Lambda_h(t) \geq \lambda_h(t)$ which is independent of ϵ .
- (II) There exists an $m > 0$ such that $\int_0^T \lambda_h(t) dt \leq C + \log(\epsilon^{-m})$ for some constant $C > 0$ independent of ϵ and we can construct a $\Lambda_h \in L_1(0, T)$ such that (4.11) holds.

Of course, Assumption 4.7(I) is a special case of Assumption 4.7(II), arising when $m = 0$. Nonetheless, when Assumption 4.7(I) is valid, the resulting a posteriori error estimates will have a more favorable dependence on the final time T than the estimates that are possible under the more general Assumption 4.7(II).

We shall prove a posteriori error estimates under the more general Assumption 4.7(II), commenting, nevertheless, on the differences that would arise in the proof under 4.7(I) instead.

4.4. Continuation argument. We begin by noting that, compared to the state-of-the-art estimates of [8, 7], there are three additional terms on the right-hand side of (4.4), (4.7), due to the use of the special test function (4.5): $\|\theta\|_{L_4(0,T;L_4(\Omega))}$ and $\|\theta_t\|_{L_4(0,T;L_4(\Omega))}$ which arise naturally and are symmetric with respect to the $\|\cdot\|_{L_4(0,T;L_4(\Omega))}$ norm that is to be estimated, while the additional term $\|\cdot\|_{L_6(0,T;L_6(\Omega))}$ can be compensated for by the presence of the additional terms $A(t)$ (weighted norms) appearing on the left-hand side. Since the $L_6(0,T;L_6(\Omega))$ -norm does not arise naturally in the Allen–Cahn energy functions, we have opted to drop the $A(t)$ terms in the analysis below.

Assuming that Λ_h is available, we set $v = \rho \in H_0^1(\Omega)$ in (4.9), to deduce

$$(4.12) \quad \begin{aligned} & \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h)\rho, \rho) \\ & \geq -\Lambda_h(t)(1 - \epsilon^2)\|\rho\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U_h)\rho, \rho). \end{aligned}$$

For $d = 2$, we work as follows. Upon setting

$$\eta_2 := \left(\frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_{PF}^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \sum_{n=1}^N \int_{J_n} (\Theta_1 + \Theta_2 + C_0(\mathcal{L}_1 + \mathcal{L}_2)) dt \right)^{1/4},$$

$\mathcal{D}_2 := \max\{4, \alpha(U_h) + 2\Lambda_h(t)(1 - \epsilon^2) + 2\}$, and $\mathcal{B}_2 := \max\{16\beta(\theta, U_h), \gamma(\theta, U_h)\}$, we use (4.12) on the left-hand side of (4.4) (we note that $-F'(U_h) \leq 1$, and ignore $\int_0^\tau A(t) dt$), to arrive at

$$\begin{aligned} & \frac{1}{4} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{\epsilon^2}{2} \int_0^\tau \|\nabla \rho\|_{L_2(\Omega)}^2 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ & \leq \eta_2^4 + \int_0^\tau \mathcal{D}_2(t) \left(\frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & \quad + \epsilon^{-6} \int_0^\tau \mathcal{B}_2(t) \left(\frac{1}{64} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \frac{1}{4} \|\rho\|_{L_2(\Omega)}^4 \right) dt \\ & \leq \eta_2^4 + \int_0^T \mathcal{D}_2(t) \left(\frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & \quad + \frac{\bar{\mathcal{B}}_2}{\epsilon^6} \sup_{t \in [0, \tau]} \left\{ \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \right\} \\ & \quad \times \left(\frac{\tau}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \sup_{t \in [0, \tau]} \frac{\tau}{2} \|\rho\|_{L_2(\Omega)}^2 \right). \end{aligned}$$

where $\bar{\mathcal{B}}_2 := \sup_{t \in [0, T]} \mathcal{B}_2(t)$.

Now, we set $E_2 := \exp(\int_0^\tau \mathcal{D}_2(t) dt)$ and, for $d = 2, 3$, we use the abbreviation

$$\begin{aligned} \mathcal{N}_{[0, \tau], d}(\rho) &:= \frac{1}{4(d-1)} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{\epsilon^2}{2} \int_0^\tau \|\nabla \rho\|_{L_2(\Omega)}^2 dt \\ & \quad + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \sup_{t \in [0, \tau]} \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \end{aligned}$$

for the collection of seminorms on the left-hand side of the last estimate. With this notation, we define the set

$$\mathcal{I}_2 := \left\{ \tau \in [0, T] : \mathcal{N}_{[0, \tau], 2}(\rho) \leq 4\eta_2^4 E_2 \right\}.$$

The set \mathcal{I}_2 is nonempty because $0 \in \mathcal{I}_2$ and the left-hand side depends continuously on τ . We set $\tau^* := \max \mathcal{I}_2$, and we assume that $\tau^* < T$; we aim to arrive at a contradiction. Hence, using the definition of the set \mathcal{I}_2 , we deduce

$$\begin{aligned} \mathcal{N}_{[0, \tau], 2}(\rho) &\leq \eta_2^4 + \int_0^\tau \mathcal{D}_2(t) \left(\frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ &\quad + 16\bar{\mathcal{B}}_2 \eta_2^8 E_2^2 (T+1) \epsilon^{-6}. \end{aligned}$$

If the last term on the right-hand side of the last estimate is bounded above by η_2^4 or, equivalently, if it holds

$$(4.13) \quad \eta_2^4 \leq \epsilon^6 (16\bar{\mathcal{B}}_2 (T+1) E_2^2)^{-1},$$

then for all $0 \leq \tau \leq \tau^*$ we have

$$\mathcal{N}_{[0, \tau], 2}(\rho) \leq 2\eta_2^4 + \int_0^\tau \mathcal{D}_2(t) \left(\frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \right) dt.$$

Since $\frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \leq \mathcal{N}_{[0, \tau], 2}(\rho)$, Grönwall's lemma implies

$$\mathcal{N}_{[0, \tau^*], 2}(\rho) \leq 2\eta_2^4 E_2$$

upon setting $\tau = \tau^*$. This contradicts the hypothesis $\tau^* < T$ and, therefore, proves that $\mathcal{I}_2 = [0, T]$.

Likewise for $d = 3$, we insert the spectral estimate (4.12) into (4.7), and we work as for $d = 2$. Setting

$$\eta_3 := \left(\frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_{PF}^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \sum_{n=1}^N \int_{J_n} (\Theta_1 + \tilde{\Theta}_2 + \tilde{C}_0(\mathcal{L}_1 + \mathcal{L}_2)) \, dt \right)^{1/4},$$

$\mathcal{D}_3 := \max\{4, \alpha(U_h) + 2\Lambda_h(t)(1 - \epsilon^2) + 3\}$, $\mathcal{B}_3 := \max\{16\tilde{\beta}(\theta, U_h), \tilde{\gamma}(\theta, U_h)\}$, and $\bar{\mathcal{B}}_3 := \sup_{t \in [0, T]} \mathcal{B}_3(t)$, $E_3 := \exp(\int_0^T \mathcal{D}_3(t) \, dt)$ through the same argumentation, we conclude that now the set $\mathcal{I}_3 := \{\tau \in [0, T] : \mathcal{N}_{[0, \tau], 3}(\rho) \leq 4\eta_3^4 E_3\}$ equals $[0, T]$ upon assuming the condition

$$(4.14) \quad \eta_3^4 \leq \epsilon^{10} (16\bar{\mathcal{B}}_3 (T+1) E_3^2)^{-1}.$$

The above argument has already confirmed the validity of the following result.

LEMMA 4.8. *Assume that (4.13) holds when $d = 2$ or (4.14) holds when $d = 3$. Then, we have the bound*

$$(4.15) \quad \mathcal{N}_{[0, T], d}(\rho) \leq 4\eta_d^4 E_d.$$

4.5. Main results. Now we are ready to present the main error estimate in the $L_4(0, T; L_4(\Omega))$ -norm, from which we can easily arrived at a fully computable a posteriori estimate in section 5.

THEOREM 4.9. *Let $u_0 \in L_\infty(\Omega)$ and $f \in L_\infty(0, T; L_4(\Omega))$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. Let u be the solution of (2.3) and U_h is its approximation (3.1), (3.6). Then, under Assumption 4.7(II) and the condition*

$$(4.16) \quad \eta_d \leq (16(T+1)\bar{\mathcal{B}}_d E_d^2)^{-1/4} \epsilon^{d-1/2},$$

the following error bound holds

$$(4.17) \quad \|u - U_h\|_{L_4(0, T; L_4(\Omega))} \leq 2\eta_d ((d-1)E_d)^{1/4} + \|\theta\|_{L_4(0, T; L_4(\Omega))}.$$

Proof. Ignoring nonnegative terms on the left-hand side of (4.15), we have

$$\|\rho\|_{L_4(0, T; L_4(\Omega))} \leq 2\eta_d ((d-1)E_d)^{1/4};$$

the proof follows by the triangle inequality. \square

Remark 4.10. Under the more restrictive Assumption 4.7(I), the continuation argument presented in section 4.4 remains analogous with minor alterations. Specifically, upon setting $m = 0$ and replacing $E_d = \exp(\int_0^T \mathcal{D}_d(t) dt)$ by $E_d = \exp(\bar{\mathcal{D}}_d T)$ with $\bar{\mathcal{D}}_d := \sup_{t \in [0, T]} \max\{4, \alpha(U_h) + 2\Lambda_h(t)(1 - \epsilon^2) + d\}$, $d = 2, 3$, Theorem 4.9 remains valid.

Remark 4.11. We stress that Theorem 4.9 also holds in cases whereby it is not possible to assume that $\|U_h\|_{L_\infty(0, T; L_\infty(\Omega))}$ is bounded independently of ϵ . We note, however, that $\|U_h\|_{L_\infty(0, T; L_\infty(\Omega))}$ remains uniformly bounded with respect to ϵ and the mesh parameters in all scenarios of practical interest we are aware of and it is typically required in scenarios ensuring the validity of Assumption 4.7.

It is instructive to discuss in detail the dependence of the various terms appearing in (4.16) and (4.17) to assess the practicality of the resulting a posteriori error bound below. The computational challenge for $\epsilon \ll 1$ is manifested by the satisfaction of the condition (4.16). Indeed as $\epsilon \rightarrow 0$ the condition (4.16) becomes increasingly more stringent to be satisfied, necessitating meshes to be increasingly locally fine enough so as to reduce the estimator η_d ; this results to proliferation of the numerical degrees of freedom. Once η_d is small enough, an adaptive algorithm could make use of Theorem 4.9 for further estimation, which requires (4.16) to be valid.

Assume for argument's sake that $\|U_h^n\|_{L_\infty(\Omega)} \leq C'$ for all $n = 1, \dots, N$ for some ϵ -independent constant $C' > 0$. Also, we have

$$\|\theta\|_{L_\infty(0, T; L_\infty(\Omega))} = \|\ell_{n-1}(t)\theta^{n-1} + \ell_n(t)\theta^n\|_{L_\infty(0, T; L_\infty(\Omega))} \leq \max_{n=1, \dots, N} \|\theta^n\|_{L_\infty(\Omega)}.$$

The $L_\infty(\Omega)$ -norm of each θ^n will be further estimated in section 5. For the moment, if also assume that $\|\theta^n\|_{L_\infty(\Omega)} \leq C'$ uniformly with respect to ϵ , then we can conclude that $2^4 \cdot 6 \leq \bar{\mathcal{B}}_d \leq CC'$, $d = 2, 3$, and, therefore,

$$3 \leq 2((T+1)\bar{\mathcal{B}}_d)^{1/4} \leq C(T+1)^{1/4}$$

for some generic constants $C > 0$, independent of ϵ , upon noting that $\sqrt[4]{6} > 1.5$.

Moreover, in the case of smooth developed interfaces (Assumption 4.7(I)), one expects that $E_d \sim 1$ as highlighted in the classical works [11, 14]. When topological changes take place, we can follow [8] and postulate that $E_d \sim \epsilon^{-m}$, $m > 0$. With the above convention, we find that (4.16) becomes

$$\eta_d \leq G_d \epsilon^{d+(m-1)/2}$$

for some constant $G_d \geq 1$ for all $m \geq 0$, thus encapsulating simultaneously both cases of Assumption 4.7.

Hence, the ϵ -dependence for the condition (4.16) appears to be *less* stringent than in the respective conditional a posteriori in the $L_\infty(L_2)$ - and $L_2(H^1)$ -norms from [5, 8, 7], which reads, roughly speaking, $\tilde{\eta} \leq c\epsilon^{4+3m}$ for the corresponding estimator $\tilde{\eta}$ and some constant $c > 0$. Therefore, seeking to prove a posteriori error estimates for the $L_4(L_4)$ -norm error is, in our view, justified, as they can be potentially used to drive space-time adaptive algorithms without excessive numerical degree of freedom proliferation. This is a significant undertaking in its own right and will be considered in detail elsewhere.

The new a posteriori error analysis appears to also improve the ϵ -dependence on the condition for the $L_2(H^1)$ - and $L_\infty(L_2)$ -norm bounds compared to [17, 5, 8, 7] in certain cases. Of course, the different method of proof above results in different terms appearing in η_d above compared to the respective conditional a posteriori error bounds from [17, 5, 8, 7]. Therefore, the performance of the proposed estimates above has to be assessed numerically before any conclusive statements can be made. In particular, we have the following result.

PROPOSITION 4.12 ($L_2(H^1)$ - and $L_\infty(L_2)$ -norm estimates). *With the hypotheses of Theorem 4.9 and, assuming condition (4.16), we have the bounds*

$$\begin{aligned} \|u - U_h\|_{L_2(0,T;H_0^1(\Omega))} &\leq 2\sqrt{2}\epsilon^{-1}\eta_d^2 E_d^{1/2} + \|\theta\|_{L_2(0,T;H_0^1(\Omega))}, \\ \|u - U_h\|_{L_\infty(0,T;L_2(\Omega))} &\leq 2\sqrt{2}\eta_d^2 E_d^{1/2} + \|\theta\|_{L_\infty(0,T;L_2(\Omega))}. \end{aligned}$$

Therefore, in the same setting as before, we have (4.16) implies

$$\eta_d^2 \leq G_d^2 \epsilon^{2d-1+m}.$$

If we accept that $\eta_d^2 \sim \tilde{\eta}$ from [5, 8, 7], for the sake of the argument, at least at the level of the conditional estimate, (4.16) gives formally favorable dependence on ϵ when $d = 2$ and $m \geq 0$ and also when $d = 3$ and $m \geq 1/2$, compared to the respective dependence $\tilde{\eta} \leq c\epsilon^{4+3m}$ from [8, 7].

5. Fully computable upper bound. The bound in Theorem 4.9 is still not fully computable, due to various terms involving θ and $\rho(0)$, which we shall now further estimate by computable quantities.

5.1. Initial condition estimates. For the terms involving $\rho(0)$, we have

$$\begin{aligned} \frac{1}{2}\|\rho(0)\|_{L_2(\Omega)}^2 &\leq \|u_0 - U_h^0\|_{L_2(\Omega)}^2 + \|\theta^0\|_{L_2(\Omega)}^2, \\ \frac{C_{PF}^2}{2}\|\rho(0)\|_{L_4(\Omega)}^4 &\leq 4C_{PF}^2(\|u_0 - U_h^0\|_{L_4(\Omega)}^4 + \|\theta^0\|_{L_4(\Omega)}^4). \end{aligned}$$

The Sobolev norms of θ appearing on η_d can be further estimated by a posteriori bounds for elliptic problems; see, e.g., [30, 1] for $p = 2$ and [27, 13, 15] for $p = \infty$. We

focus, therefore, on the derivation of the L_p -norm a posteriori error bounds for elliptic problems for θ and for θ_t via suitable duality arguments. Although the derivation is somewhat standard, we prefer to present it here with some level of detail to highlight the regularity assumptions required. Specifically, consider the dual problem

$$(5.1) \quad -\Delta z = \psi^{p-1} \quad \text{in } \Omega, \quad z = 0 \quad \text{on } \partial\Omega,$$

on an $\Omega \subset \mathbb{R}^d$ convex domain. Then, there exists a constant $C_\Omega > 0$, depending on the domain Ω , such that

$$(5.2) \quad \|z\|_{W^{2,p/(p-1)}(\Omega)} \leq C_\Omega \|\psi^{p-1}\|_{L_{p/(p-1)}(\Omega)} = C_\Omega \|\psi\|_{L_p(\Omega)}^{p-1}, \quad \text{for } p \geq 2;$$

we refer to [22] for details.

5.2. Spatial error estimates. We shall estimate Θ_2 by residual-type estimators due to the presence of non-Hilbertian norms. In view of Remark 3.2 above, $\theta^n = w^n - U_h^n$ is the error of the elliptic problem (3.3), so we can further estimate norms of θ once we have estimators of the form

$$\|\theta^n\|_{L_p(\Omega)} \leq \mathcal{E}(U_h^n, g_h^n; L_p(\Omega))$$

at our disposal for $p = 2, 4, 6$. Therefore, from (3.6) we have

$$\|\theta\|_{L_p(\Omega)} \leq \mathcal{E}(U_h^n, g_h^n; L_p(\Omega)) + \mathcal{E}(U_h^{n-1}, g_h^{n-1}; L_p(\Omega))$$

giving

$$(5.3) \quad \sum_{n=1}^N \int_{J_n} \|\theta\|_{L_p(\Omega)}^p dt \leq \hat{c} \sum_{n=1}^N k_n (\mathcal{E}^p(U_h^n, g_h^n; L_p(\Omega)) + \mathcal{E}^p(U_h^{n-1}, g_h^{n-1}; L_p(\Omega)))$$

for $\hat{c} > 0$ an algebraic constant.

Let $2 \leq p < +\infty$. To determine the estimator \mathcal{E} precisely, we set $\psi = \theta^n$ on (5.1) and we have

$$\|\theta^n\|_{L_p(\Omega)}^p = \int_{\Omega} \nabla z \cdot \nabla \theta^n dx - \int_{\Omega} \nabla \mathcal{I}_h^n z \cdot \nabla \theta^n dx = \int_{\Omega} \nabla (z - \mathcal{I}_h^n z) \cdot \nabla (\omega^n - U_h^n) dx$$

from Remark 3.2, with $\mathcal{I}_h^n : W^{1,1}(\Omega) \rightarrow V_h^n$ denoting the standard Scott–Zhang interpolation operator that satisfies optimal approximation properties [29, 4]. Continuing in standard fashion, we have

$$\begin{aligned} \|\theta^n\|_{L_p(\Omega)}^p &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla \omega^n \cdot \nabla (z - \mathcal{I}_h^n z) dx + \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \Delta U_h^n (z - \mathcal{I}_h^n z) dx \\ &\quad - \sum_{\tau \in \mathcal{T}_h^n} \int_{\partial\tau} (\nabla U_h^n \cdot \vec{n}) (z - \mathcal{I}_h^n z) ds \\ &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} r_n (z - \mathcal{I}_h^n z) dx - \sum_{e \in \mathcal{S}_h^n} \int_e \llbracket \nabla U_h^n \rrbracket (z - \mathcal{I}_h^n z) ds \\ &\leq C_{SZ} \left(\sum_{\tau \in \mathcal{T}_h^n} \|h_n^2 r_n\|_{L_p(\tau)}^p + \sum_{e \in \mathcal{S}_h^n} \|h_n^{1+1/p} \llbracket \nabla U_h^n \rrbracket\|_{L_p(e)}^p \right)^{1/p} \|z\|_{W^{2, \frac{p}{p-1}}(\Omega)} \end{aligned}$$

for some constant $C_{SZ} > 0$ independent of h_n and of the functions involved, using the approximation properties of \mathcal{T}_h^n ; here $r_n := g_h^n + \Delta U_h^n$ is the *element residual* at time t_n and $[\![\nabla U_h^n]\!]$ is the *jump* across the internal edge e . Then, the elliptic regularity estimate (5.2) implies that

$$\mathcal{E}(U_h^n, g_h^n; L_p(\Omega)) := C_\Omega C_{SZ} \left(\sum_{\tau \in \mathcal{T}_h^n} \|h_n^2 r_n\|_{L_p(\tau)}^p + \sum_{e \in \mathcal{S}_h^n} \|h_n^{1+1/p} [\![\nabla U_h^n]\!]\|_{L_p(e)}^p \right)^{1/p}.$$

For the limiting case $p = +\infty$, we can take

$$\mathcal{E}(U_h^n, g_h^n; L_\infty(\Omega)) := C_{\ell_{h,d}} \left(\sum_{\tau \in \mathcal{T}_h^n} \|h_n^2 r_n\|_{L_\infty(\tau)} + \sum_{e \in \mathcal{S}_h^n} \|h_n [\![\nabla U_h^n]\!]\|_{L_\infty(e)} \right)$$

with $\ell_{h,d} = (\ln(1/h_n))^{\alpha_d}$, where $\alpha_2 = 2$ and $\alpha_3 = 1$; we refer to [15] for details.

5.3. Mesh change estimates. The general strategy of time extensions in (3.6), (3.7) consists in decomposing θ_t as follows:

$$(5.4) \quad \theta_t = \omega_t - U_{h,t} = \frac{\omega^n - \omega^{n-1}}{k_n} - \frac{U_h^n - U_h^{n-1}}{k_n} \quad \text{for each } n = 1, \dots, N$$

with $U_h^n \in V_h^n$, $n = 1, \dots, N$. Since $V_h^n \neq V_h^{n-1}$ in general, we define the Scott–Zhang interpolation operator $\hat{\mathcal{I}}_h^n : H_0^1(\Omega) \rightarrow V_h^n \cap V_h^{n-1}$ relative to the finest common coarsening $\hat{\mathcal{T}}_h^n$ of \mathcal{T}_h^n and \mathcal{T}_h^{n-1} . The latter allows us to apply the Galerkin orthogonality property of the *elliptic reconstruction* in $V_h^n \cap V_h^{n-1}$. Moreover, we have the following approximation result: for all $e \in \hat{\mathcal{S}}_h^n \setminus \mathcal{S}_h^n$ and $1 \leq p < \infty$ it holds that

$$(5.5) \quad \|\psi - \hat{\mathcal{I}}_h^n \psi\|_{L_p(e)} \leq C_{SZ} \left(\max_{\omega(e)} \hat{h}_n \right)^{l-1/p} \|\psi\|_{W^{l,p}(\omega(e))} \quad \forall l \leq \kappa + 1,$$

where $\hat{h}_n := \max(h_n, h_{n-1})$, with $\omega(e)$ denoting the neighborhood of elements sharing the face e , where, as before, the positive constant C_{SZ} depends only on the shape regularity of the triangulation. Setting $\psi = \theta_t$ on (5.1), we work as before to deduce

$$\begin{aligned} \|\theta_t\|_{L_p(\Omega)}^p &= k_n^{-1} \int_\Omega \nabla(z - \hat{\mathcal{I}}_h^n z) \cdot \nabla(\omega^n - \omega^{n-1} - U_h^n + U_h^{n-1}) \, dx \\ &= \sum_{\tau \in \hat{\mathcal{T}}_h^n} \int_\tau \partial r_n(z - \hat{\mathcal{I}}_h^n z) \, dx - \sum_{e \in \hat{\mathcal{S}}_h^n} \int_e \partial [\![\nabla U_h^n]\!](z - \hat{\mathcal{I}}_h^n z) \, ds \end{aligned}$$

with $\hat{\mathcal{S}}_h^n$ denoting the finite element space subordinate to the coarsest common refinement $\hat{\mathcal{T}}_h^n$ of \mathcal{T}_h^n and \mathcal{T}_h^{n-1} . Standard estimation via Hölder's inequality and (5.5) give, in turn,

$$\begin{aligned} \|\theta_t\|_{L_p(\Omega)}^p &\leq \sum_{\tau \in \hat{\mathcal{T}}_h^n} \|\partial r_n\|_{L_p(\tau)} \|z - \hat{\mathcal{I}}_h^n z\|_{L_{\frac{p}{p-1}}(\tau)} + \sum_{e \in \hat{\mathcal{S}}_h^n} \|\partial [\![\nabla U_h^n]\!]\|_{L_p(e)} \|z - \hat{\mathcal{I}}_h^n z\|_{L_{\frac{p}{p-1}}(e)} \\ &\leq C_{SZ} \left(\sum_{\tau \in \hat{\mathcal{T}}_h^n} \|\hat{h}_n^2 \partial r_n\|_{L_p(\tau)}^p + \sum_{e \in \hat{\mathcal{S}}_h^n} \|\hat{h}_n^{1+1/p} \partial [\![\nabla U_h^n]\!]\|_{L_p(e)}^p \right)^{1/p} \|z\|_{W^{2, \frac{p}{p-1}}(\Omega)}. \end{aligned}$$

Finally, the assumed elliptic regularity (5.2), gives the a posteriori error estimator

$$\hat{\mathcal{E}}(U_{h,t}, g_{h,t}; L_p(\Omega)) := C_\Omega C_{SZ} \left(\sum_{\tau \in \mathcal{T}_h^n} \|\hat{h}_n^2 \partial r_n\|_{L_p(\tau)}^p + \sum_{e \in \mathcal{S}_h^n} \|\hat{h}_n^{1+1/p} \partial [\nabla U_h^n]\|_{L_p(e)}^p \right)^{1/p}$$

for which we have $\|\theta_t\|_{L_p(\Omega)}^p \leq \hat{\mathcal{E}}^p(U_{h,t}, g_{h,t}; L_p(\Omega))$.

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