

A posteriori error analysis and optimal control for phase field equations

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May, 2022

ACKNOWLEDGEMENTS

Firstly, I would like to express my sincere gratitude to my supervisors, Professors Emmanuil H. Georgoulis and Konstantinos Chrysafinos for their help and guidance during my PhD studies. They were always motivating me to be confident in my abilities and enjoy research. Without their constant support, courage and understanding it would be difficult for me to continue with the same enthusiasm and passion after 2019, the most difficult year of my life so far. Throughout these years, they were the best tutors and advisors I could hope for.

Also, special thanks go to my colleague and friend Zhaonan Dong, for spending many hours to explain difficult mathematical ideas in a fun way and for our fruitful discussions. I am also thankful for inviting me to work with him at INRIA, Paris.

Furthermore, I would like to thank my family for the unconditional love and support on every choice I made these years.

Last but not least, my deepest thanks go to Vassilis Margonis who has always been by my side not only in the joys and successes but also in the difficulties and failures just filling my life with happiness. Thanks to Vassilis, I learned to temper my pessimism and continue my life with vigour.

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CHAPTER 1

INTRODUCTION

The idea of the phase field method can be tracked back to Lord Rayleigh, Gibbs and Van der Waals and was used to describe material interfaces during phase transitions. It represents material interfaces as thin layers of finite thickness across which the properties of each material vary. This layer is referred to as the *diffuse* interface and is designed so that the exact interface lays within this thin layer; the phase field method is also known as the *diffuse interface method* in the literature.

The phase field method was initially used to model solid-liquid phase transition during which surface tension and non-equilibrium thermodynamics behavior become important at the interface. Furthermore, it is applicable to moving interface problems. In the past forty years, the phase field method has become a general methodology for moving interface problems arising in astrophysics, biology, differential geometry, image processing, multiphase fluid mechanics, chemical and petroleum engineering, materials phase transition and solidification. The common feature in the modelling of the aforementioned phenomena is the interfacial energy, which plays a crucial role in the moving interface evolutions. From the mathematical perspective, interfacial energies, such as the surface tension are often characterized by various notions of curvature of the interface, such as the mean or Gauss curvature. The latter can be conveniently expressed in terms of the phase function. As a result, the phase field method turns out to be effective for modeling the interfacial energetics, particularly the surface tension effect.

Interfaces evolving under the influence of surface tension or of some interfacial energy belong to the class of so-called *geometric moving interface problems*. The motion is driven according to some curvature-dependent geometric law that specifies the velocity V or the normal velocity V_n of the points on the interface at each given time t . The phase field formulation of these problems gives rise to interesting and challenging partial differential equations (PDE). A well known geometric moving interface problem is the *mean curvature flow*, whose governing geometric law is:

$$V \cdot n = H_{\Gamma_t},$$

where n the outward normal vector to moving interface Γ_t at time t while H_{Γ_t} stands for the mean curvature. For a recent comprehensive review of phase field models and their relationship to geometric flows, we refer to [DF20].

It is known from [ESS92] that the phase field formulation of mean curvature flow is the Allen-Cahn problem, for $\epsilon > 0$ find $u : \Omega \times (0, T] \rightarrow \mathbb{R}$, such that

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

originally introduced by Samuel M. Allen and John W. Cahn [AC79] to describe the notion of boundaries in crystalline solids. It was proposed as a simple model for the process of phase separation of a binary alloy at a fixed temperature. The boundary condition requiring the outward normal derivative to vanish on $\partial\Omega$ reflects that no mass occurs across the walls of the container Ω . The original Allen-Cahn equation from [AC79] admitted a different scaling of the time: t here, called the fast time, represents t/ϵ^2 in the original formulation. The function u represents the concentration of one of the two metallic components of the alloy.

The nonlinear function $F(s) := s^3 - s$ is the derivative of the classical *double-well potential* $\mathcal{F}(s) = (s^2 - 1)^2/4$ taking its global minimum value 0 at $s \pm 1$, i.e., satisfying $\mathcal{F}(\pm 1) = 0$, see **Figure 1**. The existence of the two stable stationary states of the Allen-Cahn problem implies that nonconvex energy is associated with the equation. Due to the nature of the non-linearity, the solution u develops time-dependent interfaces Γ_t , separating regions for which $u \approx 1$ from regions where $u \approx -1$. We can represent the aforementioned interfaces as the zero level set of the function u , $\Gamma_t := \{x \in \Omega : u(x, t) = 0\}$. Although, this does not define a sharp separation of the phases. More precisely, the phases are separated by a region of width ϵ around the zero level set of u :

$$\Gamma_t \subset Q_t := \{x \in \Omega : |u(x, t)| \leq 1 - \mathcal{O}(\epsilon)\},$$

often called *diffuse interface*. Here the parameter ϵ controls the width of *diffuse interface*. The solution moves from one region to another within the narrow *diffuse interface*. A typical example of the desired interface profile of typical solutions of the Allen-Cahn is given by

$$u(x) \approx \tanh\left(d(x)/\sqrt{2}\epsilon\right),$$

where $d(x)$ is a signed distance function between a point $x \in \Omega$ and the interface Γ_t .

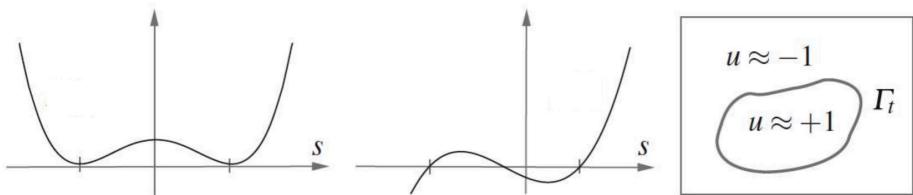


Figure 1 ([Bar16, Fig. 6.1]): Double well potential $\mathcal{F}(s) = (s^2 - 1)^2/4$ on the left and its derivative $F(s) = s^3 - s$ in the middle; solutions develop time-dependent interfaces Γ_t that separate regions in which $u(\cdot, t) \approx \pm 1$.

In addition, the Allen-Cahn equation can be interpreted as the gradient flow of the Cahn-Hilliard free-energy functional:

$$E(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{4\epsilon^2} (u^2 - 1)^2 \right) dx, \quad (1.1)$$

related to the *double-well* potential, where the first term in E is often referred to as the *bulk energy* and the second term is called the interfacial (potential) energy. Then, the Allen-Cahn equation arises as the L_2 -gradient flow

$$u_t = -E'(u), \quad (1.2)$$

where $E'(u)$ is understood as the Gâteaux derivative at u .

Another gradient flow for the same energy functional (1.1) is the Cahn-Hilliard equation

$$u_t + \Delta \left(\Delta u - \frac{1}{\epsilon^2} (u^3 - u) \right) = 0, \quad (1.3)$$

where $E'(u)$ is understood now as the Gâteaux derivative at u in the space $H^{-1}(\Omega)$. Furthermore, (1.3) stands for the phase field formulation of the Hele-Shaw flow. It was originally introduced by Cahn and Hilliard to describe the complicated phase separation and coarsening phenomena in a melted alloy that is quenched to a temperature at which only two different concentration phases can exist stably.

The Allen-Cahn equation has been studied extensively the past decades. A very important theoretical result is that the zero level set $\Gamma_t := \{x \in \Omega : u(x, t) = 0\}$ evolves according to the geometric law of mean curvature flow and Γ_t converges to the exact mean curvature flow interface as $\epsilon \rightarrow 0^+$. The rigorous justification of this limit was an open problem for a few years before been settled by Evans, Soner and Souganidis in [ESS92], who established a global result reading: for all time $t \geq 0$, the limit of zero level set of the solution of the Allen-Cahn equation is contained in the generalized solution of the motion by the mean curvature flow established in [ES91] and [CGG89]. Later, Ilmanen [Ilm93] proved that this limit is actually one of the Brakke's motion by mean curvature solution [Bra16], which is a subset of the unique generalized solution of the mean curvature flow established in [ES91] and [CGG89].

Throughout our analysis we consider that Allen-Cahn problem, that is a singularly perturbed semilinear parabolic partial differential equation (PDE), together with the following initial and boundary conditions:

$$\begin{aligned} u_t - \Delta u + \frac{1}{\epsilon^2} (u^3 - u) &= f && \text{in } \Omega \times (0, T], \\ u &= 0 && \text{on } \partial\Omega \times (0, T], \\ u(\cdot, 0) &= u_0 && \text{in } \Omega; \end{aligned} \quad (1.4)$$

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 .

The challenge of solving numerically the problem (1.4) results from the small parameter ϵ . 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 that are able to dynamically modify the local mesh size and/or the local approximation order.

The stiffness with respect to the interface length ϵ is manifested in the error analysis: deriving *a priori* and *a posteriori* error estimates which scale with low polynomial order $1/\epsilon$ is a formidable challenge. A standard error analysis of finite element approximations of (1.4) leads to *a priori* estimates with unfavorable exponential dependence on $1/\epsilon$ resulting from the application of a standard Gronwall type inequality argument. This is of limited practical value, even for moderately small interface length ϵ . The celebrated works [Che94, MS95, AF93] showed that uniform bounds for the principal eigenvalue of the linearized Allen-Cahn spatial operator about the analytical solution u , i.e.,

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

are possible as long as the evolving interface Γ_t is smooth and u has the right profile across Γ_t . Such spectral estimates are used in the seminal work [FP03] to handle the nonlinear term in the error equation and whereby *a priori* error bounds with only polynomial dependence on $1/\epsilon$ for finite element methods have been proven. The latter error estimates enabled also the proof of convergence of the numerical solutions to the solution of the mean curvature flow as mesh sizes and the parameter ϵ all tend to zero. 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 $L_2(0, T; H^1(\Omega))$ -norm, for which the condition depends only polynomially on ϵ ; this was presented in the influential works [KNS04, FW05].

This direction of research has taken a further leap forward with the seminal work [Bar05], whereby the principle eigenvalue of the linearized spatial Allen-Cahn operator *about the numerical solution*, denoted by U_h ,

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

is used instead of using *a priori* bounds for $\lambda(t)$ in an effort to arrive to fully computable *a posteriori* error estimates in $L_2(0, T; H^1(\Omega))$ - and $L_\infty(0, T; L_2(\Omega))$ -norms. By computing $\Lambda(t)$, one is able to extract important information concerning the stability of the evolution from the approximate solution. The aforementioned work is focused in the case whereby smooth evolving interfaces take place.

When the interface Γ_t undergoes topological changes, however, e.g., when an interface collapses, unbounded velocities occur and, as a result, uniform bounds concerning the principal eigenvalue break down. The key point is the postulation that the all-important principal eigenvalue λ may scale like $\lambda \sim 1/\epsilon^2$ on a time interval of length comparable to ϵ^2 . **Figure 2** depicts a typical behavior of the principal eigenvalue undergoing topological changes. This crucial observation, made in [BMO11],

showed that the principal eigenvalue can be assumed to be L_1 -integrable with respect to time variable, we may assume that there exists $m > 0$, such that the bound

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

where $x_+ := \max\{x, 0\}$ holds. Indeed, according to [Bar16, Section 6.1.4], the logarithmic term results from the transition regions in which λ grows like $1/(T_c - t)$ for a topological change that takes place at $t = T_c$. Note that this bound is affordable in order to avoid the exponential dependence on the inverse of the interface length in the resulting estimates.

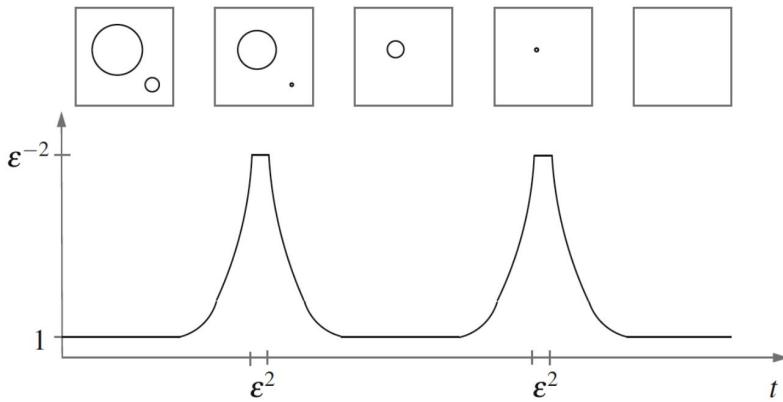


Figure 2 ([Bar16, Fig. 6.5]): Two topological changes in an evolution defined by the Allen–Cahn equation; the topological changes are accompanied by extreme principal eigenvalues; the eigenvalue increases like $1/(T_c - t)$ before a topological change occurs at T_c .

The subsequent works [BM11, BMO11] consider the more realistic scenario when topological changes occur and postulate the above assumption regarding the principal eigenvalue to derive robust conditional *a posteriori* error analysis under topological changes in $L_2(0, T; H^1(\Omega))$ - and $L_\infty(0, T; L_2(\Omega))$ -norms. Furthermore, in [BM11], the authors combine the elliptic reconstruction framework, that is initially proposed in [MN03, LM06] with techniques developed in [BMO11] to derive robust and quasi-optimal *a posteriori* error estimates in $L_\infty(0, T; L_2(\Omega))$ -norm. We refer also [GLV11, CGM13] for application of elliptic reconstruction to non-conforming methods. We also mention [GM13] whereby *a posteriori* error bounds in the $L_\infty(0, T; L_r(\Omega))$ -norms, $r \in [2, \infty]$ for the semidiscrete Allen-Cahn problem are proved.

In a recent work [Chr19], *a priori* bounds for the $L_4(0, T; L_4(\Omega))$ -norm error are proved, which appear to deliver a rather favourable $1/\epsilon$ -polynomial dependence on the respective constant, noting that $L_4(0, T; L_4(\Omega))$ -norm is present in the stability of the spatial Allen-Cahn operator upon multiplication of (1.4) by u and integration with respect to space and to time. The importance of the $L_4(0, T; L_4(\Omega))$ -norm is evidenced upon interpreting the Allen-Cahn equation as a gradient flow of the Cahn-Hilliard free-energy functional (1.2). Upon observing the different scaling with respect to ϵ , it is evident that the quantity $(1/\epsilon^2)\|u\|_{L_4(\Omega)}^4$ plays a crucial role. An immediate question is whether proving conditional type *a posteriori* error bounds in

$L_4(0, T; L_4(\Omega))$ -norm can also improve the dependence of the condition on the interface length ϵ .

Motivated by the observation that $L_4(0, T; L_4(\Omega))$ -norm may offer favorable $1/\epsilon$ -dependence, we manage to prove conditional type *a posteriori* error bounds in the $L_4(0, T; L_4(\Omega))$ -norm for fully discrete approximations of (1.4). The numerical scheme consists of the backward Euler method in time combined with conforming finite elements method in space. The finite element space is allowed to change between time steps. This work is published in [CGP20] and is presented in detail in Chapter 3. The key result is the reduced ϵ -dependence of the conditional assumption regarding our total estimator η_d for $d \in \{2, 3\}$, which reads

$$\eta_d \leq G_d \epsilon^{d+(m-1)/2}, \quad (1.5)$$

for some constant $G_d \geq 1$ and for all $m \geq 0$. In particular, the ϵ -dependence of (1.5) appears to be less stringent than in the respective conditional *a posteriori* estimate in the $L_\infty(0, T; L_2(\Omega))$ - and $L_2(0, T; H^1(\Omega))$ -norms from [Bar05, BM11, BMO11] 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 $L_4(0, T; L_4(\Omega))$ -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. It is of crucial importance that the results are valid under the hypothesis of the existence of a spectral estimate under topological changes in the spirit of [BMO11].

The *a posteriori* analysis in Chapter 3 is based on a carefully constructed non-standard test function that gives rise to the $\|\cdot\|_{L_4(0,T;L_4(\Omega))}^4$ norm for the quantities requiring estimation. A key attribute of the new testing is that leading order time- and space-error terms appear inside $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$ norms. The discrepancy in powers between the error norm, $\|\cdot\|_{L_4(0,T;L_4(\Omega))}^4$, and the estimator norms, $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$, leads to the various $1/\epsilon$ -dependent constants in the estimators to have formally milder conditions ensuring the validity of the *a posteriori* error bounds.

Since, the $L_4(0, T; L_4(\Omega))$ -norm is weaker than $L_2(0, T; H^1(\Omega))$ -norm, we avoid the direct approach techniques that estimate the difference of the exact solution and the numerical approximation. Instead, the argumentation consists of splitting the total error into two parts using a new variant of the *elliptic reconstruction* technique introduced in [GLW21], as well as known ideas regarding time reconstruction from [NSV00, MN06, LM06]. In this vein, each error term can be bounded separately. Due to the use of the elliptic reconstruction technique, we can use any available residual-based *a posteriori* error estimates for elliptic problems in various norms to control the main part of the spatial error, that is the *elliptic reconstruction* error. In the context of finite element method (FEM), the theory of the *a posteriori* estimates for linear elliptic problems is mature [Ver99, AO00]. As for the second part of the error, it satisfies a modified parabolic PDE with a right-hand side that can be monitored in an *a posteriori* fashion. Using non-standard energy and continuation arguments, we are able to derive the desired estimates. At the same time, the 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. As a result of the method of proof, the new *a posteriori* error analysis provides also $L_\infty(0, T; L_2(\Omega))$ - and $L_2(0, T; H^1(\Omega))$ -norm *a posteriori* error bounds, which appear to be valid under a less stringent smallness condition compared to the aforementioned results from the literature, at least in certain regimes.

The second main contribution of this work is the extension of the *a posteriori* error analysis to the case of a space-time discontinuous Galerkin method of arbitrary order allowing, in particular, the space discretization to consist of very general polygonal ($d = 2$) or polyhedral ($d = 3$) element shapes. Specifically, we consider hp -version discontinuous Galerkin time-stepping, in conjunction with interior penalty discontinuous Galerkin method (IPDG) in space. The *a posteriori* error bounds are proven for meshes consisting of very general polygonal and polyhedral element shapes in two and three dimensions in space, respectively. In particular, arbitrary number of very small faces are allowed on each polygonal/polyhedral element. We shall, henceforth, refer to these elements as *polytopes*. The only (very mild) condition on the mesh is the existence of a subdivision of finite non-overlapping star-shaped polytopic sub-elements per element, in addition to certain mild shape regularity assumptions, inspired from [CDG21], trace and inverse estimates that are adapted to the mesh properties. The above results are presented in detail in Chapter 4.

The main skeleton of the proof is analogous to the proving steps in Chapter 3. Again, we avoid the straightforward approach for the error analysis. We split the total error using a *space-time reconstruction*, constructed as the *time reconstruction of elliptic reconstruction*. The dG-time stepping reconstruction was initially proposed in [MN06] and further studied in [SW10, HW17]. Thus, the total error is decomposed into two terms that can be bounded separately. The main focus is to bound from above by fully computable quantities the error term that is continuous with respect to time variable. To do so, we seek for an error equation, which is a modified parabolic PDE and then through suitable energy and continuation arguments, we arrive to a right-hand side consisting of terms that may be controlled in an *a posteriori* fashion. The second part of the error decomposition can be interpreted as the *time reconstruction* and the *space reconstruction errors* which are following the ideas from [GLW21].

The *space reconstruction* error should be incorporated as the error of the elliptic problem whose weak solution is the *elliptic reconstruction*. The main difficulty that we need to overcome is the lack of the orthogonality property of the *elliptic reconstruction* error that is an immediate consequence of the inconsistency of the extension of the spatial dG-bilinear form with respect to the elliptic problem that admits *elliptic reconstruction* as a weak solution. To that end, we introduce a variant of the concept of the orthogonality of the *elliptic reconstruction* error in the dG-spaces. Moreover, we prove approximation estimates for linear elementwise discontinuous functions with fully explicit computable constants that are, in turn, required for the proof of new elliptic *a posteriori* error estimators in $L_p(\Omega)$ -norms, $p \geq 2$, for IPDG on polytopic meshes.

The last contribution of this work is the analysis and numerical approximation of an optimal control problem related to the Allen-Cahn problem and are presented in Chapters 5 and 6, respectively. This work is already submitted for publication [CP22]. From now on, in keeping with the notational traditional of literature, we adopt the following notation: we refer to y as the solution to the Allen-Cahn problem while the forcing term f in (1.4) is substituted by the control denoted by u . We consider the distributed optimal control problem that is governed by the Allen-Cahn equation:

$$\begin{aligned} J(u) = & \frac{1}{2} \int_0^T \int_{\Omega} |y_u(t, x) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_{\Omega} |y_u(T, x) - y_{\Omega}(x)|^2 dx \\ & + \frac{\mu}{2} \int_0^T \int_{\Omega} |u(t, x)|^2 dx dt, \end{aligned} \tag{1.6}$$

subject to

$$\begin{aligned} y_{u,t} - \Delta y_u + \frac{1}{\epsilon^2}(y_u^3 - y_u) &= u && \text{in } \Omega_T = \Omega \times (0, T), \\ y_u &= 0 && \text{on } \Sigma_T = \partial\Omega \times (0, T), \\ y_u(\cdot, 0) &= y_0 && \text{in } \Omega. \end{aligned} \tag{1.7}$$

In particular, our goal is to intervene to the dynamics of (1.7) by using a control function u , in order to guarantee that the solution y_u will be as close as possible to a given target y_d . Here $\mu > 0$ is the typical Tikhonov regularization term, while the inclusion of the terminal tracking term in the functional (with $\gamma \geq 0$) is necessary in order to obtain effective approximations near the end point of the time interval. Throughout this work, the set of admissible controls is defined as

$$U_{ad} = \left\{ u \in L_2(0, T; L_2(\Omega)) ; u_a \leq u(t, x) \leq u_b \text{ for a.e. } (t, x) \in \Omega_T \right\},$$

and the optimal control problem is formulated, in the standard reduced functional form, as

$$\begin{cases} \min J(u) \\ u \in U_{ad}. \end{cases} \tag{1.8}$$

Note that the above optimal control problem is non-convex. Thus, it is necessary to distinguish between local and global solutions. A control $\bar{u} \in U_{ad}$ is said to be a local optimal control of (1.8) in the sense of $L_2(0, T; L_2(\Omega))$, if there exists $\alpha > 0$ such that $J(\bar{u}) \leq J(u)$ for all $u \in U_{ad} \cap B_\alpha(\bar{u})$, where $B_\alpha(\bar{u})$ is the open ball of $L_2(0, T; L_2(\Omega))$ centered at \bar{u} with radius α .

Optimal control problems having states constrained to semilinear parabolic PDEs have been extensively studied. We refer the reader to [Trö10], see also references therein for an overview of optimal control problems related to classical elliptic and parabolic semilinear PDEs. In fact, various issues such as existence, first and second order necessary and sufficient conditions have been considered even for nonstandard optimal control problems related to semilinear parabolic PDEs: see for instance [CKK17] BV controls, [CMR19] for control problems in absence of Tikhonov regularization term, [CHW17, CRT15, CRT18, CT19] (and references therein) for control problems with sparse controls, and [MS17] for control problems for non smooth semilinear parabolic PDEs.

The numerical analysis of optimal control problems with semilinear parabolic PDEs as constraints have been considered in [NV12] for control constraints with piecewise constants / linear controls / variational discretization approach, in [CK12] for discontinuous in time schemes, no constraints, and in [CMR19] whereby error estimates in absence of Tikhonov term are proved. In these works, error estimates of fully-discrete approximations have been presented under a monotonicity assumption on the semilinear term. In [CC12, CC14, CC16, CC17] the numerical analysis of optimal control problems related to the evolutionary Navier-Stokes equations, including error estimates are presented. Finally, for related works for other nonlinear parabolic PDEs, we refer the reader to cite [GHK19] for time-discrete two-phase flows, [HK21] for a POD approach for quasilinear parabolic PDEs and to [HR21] for *a priori* estimates for a coupled semilinear PDE-ODE system.

A common ingredient in the error analysis of fully-discrete schemes for optimal control problems related to nonlinear parabolic PDEs, under control constraints, e.g.,

[NV12, CMR19, CC12, CC14, CC16, CC17, HR21], is the use of results regarding the Lipschitz continuity of the control to state and of state to adjoint mappings, the derivation of first and second order necessary and sufficient optimality conditions, and detailed error estimates of the corresponding control to state, and state to adjoint mappings that allow the classical *localization* argument of [ACT02, CMT05, CR06, CMR07] (developed for error analysis of discretization schemes for semilinear elliptic PDE constrained optimization problems) to work under the prescribed regularity assumptions.

However, to our best knowledge none of the above key results include the case of the Allen-Cahn equation. For instance, the Allen-Cahn involves an nonmonotone nonlinearity that satisfies $\frac{1}{\epsilon^2} F'(s) := \frac{1}{\epsilon^2} (3s^2 - 1) \geq -\frac{1}{\epsilon^2}$. As a consequence, for realistic values of ϵ the *classical* approaches for proving the Lipschitz continuity of the control to state mapping as well as its numerical analysis, fail since they introduce constants depending exponentially upon $\frac{1}{\epsilon^2}$. As discussed above, for the numerical analysis of the uncontrolled Allen-Cahn equation, i.e. for $u = 0$, this difficulty is circumvented in the literature [FP03, KNS04, FW05, BMO11, BM11], where *a priori* and *a posteriori* error estimates were established for the homogeneous Allen-Cahn equation with constants that dependent polynomially upon $1/\epsilon$ based on suitable approximation of the *spectral estimate* and a nonstandard continuation argument of the form of a nonlinear Gronwall Lemma. Unfortunately, such analysis typically requires regularity assumptions on both state and adjoint variables as well as to their fully-discrete counterparts that are not available within the optimal control context. For example, the assumption $y \in L_\infty(0, T; H^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap H^2(0, T; L_2(\Omega))$, used in the above mentioned works for *a priori* estimates of the uncontrolled Allen-Cahn equation, is not realistic in our optimal control setting. In addition, similar difficulties arise when dealing with analysis and numerical analysis of the state to adjoint mapping. In fact, it turns out that the analysis can be further complicated due to the absence of the cubic nonlinear term that generates the $L_4(0, T; L_4(\Omega))$ norm when testing (1.7) with y .

The approach of our analysis avoids the construction of any discrete approximation of a spectral estimate and assumptions about pointwise space-time bounds of fully discrete solution of the control to state mapping. Indeed, we apply the spectral estimate only in ‘continuous level’ and all of our results admit the regularity imposed of the optimal control setting. In Chapter 5 we study both control to state and state to adjoint mappings in order to derive first and second order optimality conditions. The main concern is to use techniques that allow the derivation of Lipschitz constant which do not exhibit exponentially dependence on $1/\epsilon$. We manage to prove Lipschitz continuity results of control to state mapping with Lipschitz constants being independent of $1/\epsilon$ as long as a closeness assumption among control functions holds. As for the state to adjoint mapping, we employ the Lipschitz continuity result of the control to state mapping and stability results to deduce Lipschitz constants that depend at least polynomially on $1/\epsilon$.

The numerical approximation of the optimal control problem in Chapter 6 considers a fully discrete scheme that combines discontinuous Galerkin dG(0) in time and lowest order finite element method in space. We begin with the numerical analysis of the control to state mapping. In particular, we derive *a priori* error bounds using a carefully constructed globally space-time projection, discrete stability results and a generalized discrete Gronwall lemma. The derivation of error estimates of the discrete state to adjoint mapping is a challenging proof that requires a lot of technical intermediate steps. Specifically, we need to prove beforehand discrete stability results using a pseudo duality and a boot-strap argumentation. Finally, we combine all

the above results to prove estimates of the difference between local optimal controls and their discrete approximations and also estimates for the differences between the corresponding state and adjoint state and their discrete approximations.

CHAPTER 2

PRELIMINARIES

In this chapter, we provide the necessary notation, definitions, as well as some technical results that will be useful below.

2.1 Sobolev spaces

Given a multi-index $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$, $d \geq 1$ of length $|\alpha| := \alpha_1 + \dots + \alpha_d$, we consider

$$D^\alpha = \left(\frac{\partial}{\partial x_1} \right)^{\alpha_1} \cdots \left(\frac{\partial}{\partial x_1} \right)^{\alpha_d} = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}.$$

Let Ω be bounded open subset of the Euclidean space \mathbb{R}^d with boundary $\partial\Omega$. For $k \in \mathbb{N}$, we denote by $C^k(\Omega)$ the set of all continuous functions, v , defined on Ω such that $D^\alpha v$ are continuous on Ω for all $|\alpha| \leq k$. In particular, for $k = 0$ we simply write $C(\Omega)$. Furthermore, let $C_0^\infty(\Omega)$ the set of functions in $C^k(\Omega)$ that have compact support in Ω .

Next, we introduce the notion of the weak derivative that is necessary to define the Sobolev space. Suppose that $u, \omega \in L_1^{\text{loc}}(\Omega)$. We say that ω is the α -th derivative of u , if

$$\int_{\Omega} u D^\alpha \varphi \, dx = (-1)^{|\alpha|} \int_{\Omega} \omega \varphi \, dx \quad \forall \varphi \in C_0^\infty(\Omega).$$

In other words, if there exists a function ω which verifies the above equality for all φ , we say $D^\alpha u = \omega$ in the weak sense.

We denote by $L_p(\Omega)$, $1 \leq p \leq \infty$ the standard Lebesgue spaces of real valued functions with corresponding norms $\|\cdot\|_{L_p(\Omega)}$,

$$\|v\|_{L_p(\Omega)} := \left(\int_{\Omega} |v(x)|^p \, dx \right)^{1/p}, \quad p \in [1, +\infty), \quad \|v\|_{L_\infty(\Omega)} := \text{ess. sup}_{x \in \Omega} |v(x)|.$$

Definition 2.1. Let k be a non-negative integer. We define the k th order of Sobolev space based on $L_p(\Omega)$, as

$$W^{k,p}(\Omega) := \{v \in L_p(\Omega) : D^\alpha v \in L_p(\Omega), |\alpha| \leq k\},$$

equipped with the associated norm and seminorm:

$$\|v\|_{W^{k,p}(\Omega)} := \left(\sum_{|\alpha| \leq k} \|D^\alpha v\|_{L_p(\Omega)}^p \right)^{1/p}, \quad |v|_{W^{k,p}(\Omega)} := \left(\sum_{|\alpha|=k} \|D^\alpha v\|_{L_p(\Omega)}^p \right)^{1/p},$$

for $p \in [1, +\infty)$; for $p = \infty$, we require instead that

$$\|v\|_{W^{k,\infty}(\Omega)} := \max_{|\alpha| \leq k} \|D^\alpha v\|_{L_\infty(\Omega)}, \quad |v|_{W^{k,\infty}(\Omega)} := \max_{|\alpha|=k} \|D^\alpha v\|_{L_\infty(\Omega)},$$

are finite.

For $p = 2$, the space $W^{k,2}(\Omega)$ is a Hilbert space with the inner product

$$(u, v)_{W^{k,2}(\Omega)} := \sum_{|\alpha| \leq k} (D^\alpha u, D^\alpha v),$$

and we shall use the notation $H^k(\Omega) := W^{k,2}(\Omega)$, $k \geq 0$. Throughout, the analysis we shall frequently refer to the Hilbertian Sobolev spaces $H^1(\Omega)$ and $H^2(\Omega)$;

$$H^1(\Omega) = \left\{ v \in L_2(\Omega) : \frac{\partial v}{\partial x_j} \in L_2(\Omega), 1 \leq j \leq d \right\},$$

with norm

$$\|v\|_{H^1(\Omega)} = \left\{ \|v\|_{L_2(\Omega)}^2 + \sum_{j=1}^d \left\| \frac{\partial v}{\partial x_j} \right\|_{L_2(\Omega)}^2 \right\}^{1/2},$$

and

$$H^2(\Omega) = \left\{ v \in L_2(\Omega) : \frac{\partial v}{\partial x_j}, \frac{\partial^2 v}{\partial x_i \partial x_j} \in L_2(\Omega), 1 \leq i, j \leq d \right\},$$

with norm

$$\|u\|_{H^2(\Omega)} = \left\{ \|u\|_{L_2(\Omega)}^2 + \sum_{j=1}^d \left\| \frac{\partial u}{\partial x_j} \right\|_{L_2(\Omega)}^2 + \sum_{i,j=1}^d \left\| \frac{\partial^2 u}{\partial x_i \partial x_j} \right\|_{L_2(\Omega)}^2 \right\}^{1/2}.$$

Furthermore, we define the closed subspace of $H^1(\Omega)$:

$$H_0^1(\Omega) := \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\},$$

which is also a Hilbert space, with the same norm and inner product as $H^1(\Omega)$; the notation $u|_{\partial\Omega} = 0$ is understood in the sense of the traces of functions in Sobolev spaces. We refer to [Eva98, Sections 5.2 and 5.5] for the understanding of the Sobolev spaces and the notion of the trace operator, respectively.

We consider henceforth two (real) Hilbert spaces H and V such that H is identified with his own dual, $H' \equiv H$, and the embedding $V \subset H$ is continuous and dense. The triple:

$$V \subset H \subset V', \tag{2.1}$$

is called an *evolution triple* or a *Gelfand's triple*; here V' denotes the dual space of V with respect to the pivot space H . Owing to the Riesz Representation Theorem, functionals $F \in V'$ can be continuously extended to the larger space H if and only if they are of the form

$$F(v) = (f, v)_H \quad \forall v \in V,$$

with a fixed $f \in H$, see, e.g., [Rou13, Chapter 7.2]. We introduce $H^{-1}(\Omega)$ as the dual space of $H_0^1(\Omega)$, reading $(H_0^1(\Omega))' = H^{-1}(\Omega)$, endowed with the norm

$$\|v\|_{H^{-1}(\Omega)} = \sup \left\{ \langle v, v \rangle : v \in H_0^1(\Omega), \|v\|_{H_0^1(\Omega)} \leq 1 \right\}.$$

In the case of $V = H_0^1(\Omega)$ and $H = L_2(\Omega)$, the duality pairing $\langle \cdot, \cdot \rangle$ between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$ can be extended to the standard L_2 -inner product denoted by (\cdot, \cdot) . Indeed, for $f \in L_2(\Omega)$ and for $v \in V$, we have

$$\langle f, v \rangle = (f, v).$$

Theorem 2.2 (Sobolev Embedding). Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $1 < p < \infty$. Then, the following embedding exists and is continuous:

$$W^{1,p}(\Omega) \subset L_{p^*}(\Omega), \tag{2.2}$$

provided the exponent p^* is defined as

$$p^* := \begin{cases} \frac{dp}{d-p} & \text{for } p < d, \\ +\infty & \text{for } p > d, \\ [p, +\infty) & \text{for } p = d, \end{cases}$$

see, e.g., [Rou13, Theorem 1.20].

2.2 Bochner spaces

The concept of functions with values in Banach spaces is a fundamental tool for the treatment of evolution problems. Let X be any Banach space. We now switch our viewpoint, by associating with v a mapping

$$v : [0, T] \rightarrow X,$$

defined by

$$[v(t)](x) := v(t, x), \quad x \in \Omega, 0 \leq t \leq T.$$

In other words, we consider v not as a function of x and t together, but rather as a mapping u of t into the space X of functions of x . We refer to [Eva98, Section 5.9.2] or [Rou13, Chapter 7] for more details about spaces involving time.

Definition 2.3. We denote by $L_p(0, T; X)$, $1 \leq p < \infty$, the linear space of all measurable vector-valued functions $v : [0, T] \rightarrow X$ having the property

$$\int_0^T \|v(t)\|_X^p dt < \infty.$$

The space $L_p(0, T; X)$ is a Banach space with respect to the norm

$$\begin{aligned}\|v\|_{L_p(0, T; X)} &= \left(\int_0^T \|v\|_X^p dt \right)^{1/p}, \quad p \in [1, +\infty), \\ \|v\|_{L_\infty(0, T; X)} &= \text{ess. sup}_{t \in [0, T]} \|v\|_X.\end{aligned}$$

We denote by $C(0, T; X)$ the space consisting of all continuous functions

$$v : [0, T] \rightarrow X,$$

with

$$\|v\|_{C(0, T; X)} := \max_{t \in [0, T]} \|v\|_X < \infty.$$

Observe that for $1 \leq q \leq p \leq \infty$

$$C(0, T; X) \subset L_p(0, T; X) \subset L_q(0, T; X).$$

Definition 2.4. We denote by $W(0, T)$ the linear space of all $v \in L_2(0, T; X)$ having a weak (temporal) derivative $v_t \in L_2(0, T; X')$, equipped with the norm

$$\|v\|_{W(0, T)} = \left(\int_0^T \|v(t)\|_X^2 + \|v_t(t)\|_{X'}^2 dt \right)^{1/2}.$$

Consider a *Gelfand triple* $X \subset H \subset X'$. Then, every $v \in W(0, T)$ coincides, possibly after suitable modifications on a set of zero measure, with an element of $C(0, T; H)$. In this sense, we have the continuous embedding $W(0, T) \hookrightarrow C(0, T; H)$.

2.3 Useful inequalities

We shall use extensively some classical inequalities throughout the analysis.

Gagliardo-Nirenberg-Ladyzhenskaya interpolation inequalities (GNL): For all $v \in H_0^1(\Omega)$, there exists $\tilde{c} > 0$ independent of v such that

$$\|v\|_{L_4(\Omega)} \leq \tilde{c} \|v\|_{L_2(\Omega)}^{1/2} \|\nabla v\|_{L_2(\Omega)}^{1/2}, \quad \text{for } d = 2, \quad (2.3)$$

$$\|v\|_{L_3(\Omega)} \leq \tilde{c} \|v\|_{L_2(\Omega)}^{1/2} \|\nabla v\|_{L_2(\Omega)}^{1/2}, \quad \text{for } d = 3, \quad (2.4)$$

$$\|v\|_{L_4(\Omega)} \leq \tilde{c} \|v\|_{L_2(\Omega)}^{1/4} \|\nabla v\|_{L_2(\Omega)}^{3/4}, \quad \text{for } d = 3, \quad (2.5)$$

see, e.g., [Rou13, Theorem 1.24].

Hölder inequality: Let $p, q \in [1, +\infty]$. Then, for any $v \in L_p(\Omega)$ and $u \in L_q(\Omega)$, we have

$$|(v, u)| \leq \|v\|_{L_p(\Omega)} \|u\|_{L_q(\Omega)}, \quad (2.6)$$

where q is the so-called conjugate exponent defined by:

$$q := \begin{cases} p/(p-1) & \text{for } 1 < p < +\infty, \\ 1 & \text{for } p = +\infty, \\ +\infty & \text{for } p = 1. \end{cases}$$

In addition, Hölder inequality allows for an interpolation between $L_{p_1}(\Omega)$ and $L_{p_2}(\Omega)$: for $p_1, p_2, p \in [1, +\infty]$ and $m \in [0, 1]$, we have

$$\|v\|_{L_p(\Omega)} \leq \|v\|_{L_{p_1}(\Omega)}^m \|v\|_{L_{p_2}(\Omega)}^{1-m}, \quad \text{where } \frac{m}{p_1} + \frac{1-m}{p_2} = \frac{1}{p}. \quad (2.7)$$

Poincaré inequality: Let $1 \leq p < \infty$ and let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Then, there exists a constant C_P , depending on Ω and p such that, for every function $v \in W_0^{1,p}(\Omega)$, we have

$$\|v\|_{L_p(\Omega)} \leq C_P \|\nabla v\|_{L_p(\Omega)}. \quad (2.8)$$

Poincaré inequalities are very useful tool in our analysis. A prototype is due to Wirtinger in its simplest form, bounds the L_p -norm of a function with mean value 0 of the L_p -norm of its gradient and a constant depending solely on the domain Ω . In other words, if $\bar{v} = |\Omega|^{-1} \int_{\Omega} v \, dx$ is the average of v in Ω and $\text{diam}(\Omega)$ denotes the diameter of Ω ; then

$$\bar{C}_p(\Omega) = \sup_{v \in W^{1,p}(\Omega)} \frac{\|v - \bar{v}\|_{L_p(\Omega)}}{\text{diam}(\Omega) \|\nabla v\|_{L_p(\Omega)}} \quad (2.9)$$

is finite under appropriate conditions on Ω . If one considers the class of convex domains denoted by \mathcal{C} , sharp uniform bounds of the Poincaré constants are known. More precisely, setting $\bar{C}_p = \sup_{\Omega \in \mathcal{C}} \bar{C}_p(\Omega)$, recent results [AD04] and [CW06b] show that

$$\bar{C}_1 = \frac{1}{2}, \quad \bar{C}_2 = \frac{1}{\pi}, \quad \bar{C}_p \leq 2 \left(\frac{p}{2} \right)^{1/p}.$$

Furthermore, several explicit upper bounds for Poincaré constants of not necessarily convex domains, focusing on finite element stars are proven in [VV11].

Young's inequality: For any $\delta > 0$, $a, b \geq 0$, $p, q > 1$ and for some $C(p, q) > 0$, it holds

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

Gronwall inequalities: We recall that the continuous Gronwall lemma states that if a nonnegative function $v \in C(0, T)$ satisfies

$$v(s) \leq A + \int_0^s \alpha(t) v(t) \, dt,$$

for all $s \in [0, T]$, with a nonnegative function $\alpha \in L_1(0, T)$, then there holds that

$$v(t) \leq A \exp \left(\int_0^T \alpha(t) \, dt \right).$$

The discrete analogue states: suppose that the nonnegative sequence $\{v^n\}_{n=1}^m$ satisfies

$$v^m \leq A + k \sum_{n=1}^m \alpha_n v^n$$

for all $0 \leq m \leq N$ and if $k\alpha_n \leq 1/2$ for $n = 1, 2, \dots, N$, then we have that

$$\sup_{1 \leq n \leq N} v^n \leq A \exp \left(2k \sum_{n=1}^N \alpha_n \right).$$

The condition $k\alpha_n \leq 1/2$ is required to absorb the term $\alpha_m v^m$.

We include generalizations of the continuous and the discrete Gronwall lemma that are required for the upcoming analysis since they allow an additional super-linear term to be controlled as long as the function or the sequence remains sufficiently small. The proofs of the above two lemmas are presented in detail in [Bar16, Section 6]. The proof of the continuous lemma is adapted from [KNS04] while a similar result can be found in [FW05]. The proof of the discrete analogue is adapted from [FP03].

Lemma 2.5. [Bar16, Proposition 6.2] Let the nonnegative functions $w_1 \in C(0, T)$, $w_2, w_3 \in L_1(0, T)$, $\alpha \in L_\infty(0, T)$ and the real number $A \geq 0$ that satisfy for all $t \in [0, T]$,

$$w_1(t) + \int_0^t w_2(s) \, ds \leq A + \int_0^t \alpha(s) w_1(s) \, ds + \int_0^t w_3(s) \, ds.$$

Assume that for $B \geq 0$, $\beta > 0$ and every $t \in [0, T]$, it holds that

$$\int_0^t w_3(s) \, ds \leq B \sup_{s \in [0, t]} w_1^\beta(s) \int_0^t (w_1(s) + w_2(s)) \, ds.$$

Set $E := \exp \left(\int_0^T \alpha(t) \, dt \right)$ and assume that $4AE \leq (4B(T+1)E)^{-1/\beta}$. Then, it yields that

$$\sup_{t \in [0, T]} w_1(t) + \int_0^T w_2(t) \, dt \leq 4AE.$$

Lemma 2.6. [Bar16, Lemma 6.2] Let $k > 0$ and suppose that the nonnegative real sequences $\{w_j^n\}_{n=0}^N$, $j = 1, 2, 3$, $\{\alpha^n\}_{n=0}^N$ and the real number $A \geq 0$ satisfy

$$w_1^m + k \sum_{n=1}^m w_2^n \leq A + k \sum_{n=1}^m \alpha^n w_1^n + k \sum_{n=1}^{m-1} w_3^n,$$

for all $m = 1, \dots, N$, that $\sup_{n=1, \dots, N} k\alpha^n \leq 1/2$ and $Nk \leq T$. Assume that for $B \geq 0$, $\beta > 0$ and every $m = 1, \dots, N$ we have

$$k \sum_{n=1}^{m-1} w_3^n \leq B \sup_{n=1, \dots, m-1} (w_1^n)^\beta k \sum_{n=1}^{m-1} (w_1^n + w_2^n).$$

Set $E := \exp \left(2k \sum_{n=1}^N \alpha^n \right)$ and assume that $4AE \leq (4B(T+1)E)^{-1/\beta}$. Then, we obtain

$$\sup_{n=1, \dots, N} w_1^n + k \sum_{n=1}^N w_2^n \leq 4AE.$$

CHAPTER 3

BACKWARD EULER - FINITE ELEMENT METHOD

This chapter 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 consists of 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 interface length ϵ . The results hold when the evolving interfaces are smooth and when they undergo topological changes. The derivation relies crucially on the availability of a spectral estimate for the linearized Allen-Cahn operator about the approximate 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 $L_2(0, T; H^1(\Omega))$, $L_\infty(0, T; L_2(\Omega))$ -norms in certain regimes, at least formally in the level of the ϵ -dependence of the conditional assumption.

3.1 Weak formulation

The following weak formulation of (1.4) will be used subsequently. Assume that $f \in L_\infty(0, T; L_4(\Omega))$ and $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$. Then, for all $v \in H_0^1(\Omega)$ and 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

$$\begin{aligned} \langle u_t(t), v \rangle + (\nabla u(t), \nabla v) + \epsilon^{-2} (u^3(t) - u(t), v) &= \langle f(t), v \rangle, \\ (u(0), v) &= (u_0, v). \end{aligned} \quad (3.1)$$

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

$$\begin{aligned} (u(T), v(T)) + \int_0^T \left(-\langle u, v_t \rangle + (\nabla u, \nabla v) + \epsilon^{-2}(u^3 - u, v) \right) dt \\ = (u_0, v(0)) + \int_0^T \langle f, v \rangle dt, \end{aligned} \quad (3.2)$$

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

3.2 The fully discrete scheme and reconstructions

We first present the fully discrete scheme for the Allen-Cahn problem (1.4) and we define suitable space and time reconstructions of the fully discrete scheme.

3.2.1 Discretization

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

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 meshsize function, $h_n : \Omega \rightarrow \mathbb{R}$, by $h_n(x) := \text{diam}(\tau)$, $x \in \tau$ for $\tau \in \mathcal{T}_h^n$. We shall refer to $\tau \in \mathcal{T}_h^n$ as elements, with the following properties:

- (i) $\bar{\Omega} = \cup_{\tau \in \mathcal{T}_h^n} \bar{\tau}$, denoting by $\bar{\cdot}$ the closure of a set in \mathbb{R}^d ;
- (ii) for $\tau, \tau' \in \mathcal{T}_h^n$, we only have the possibilities: either $\tau = \tau'$, or $\bar{\tau} \cap \bar{\tau}'$ is a common (whole) $(d-r)$ -dimensional face with $1 \leq r < d$ (i.e., face, edge or vertex, respectively).

To each \mathcal{T}_h^n we associate the finite element space:

$$V_h^n := \{\chi \in C(\bar{\Omega}); \chi|_\tau \in \mathbb{P}_\kappa(\tau) \quad \forall \tau \in \mathcal{T}_h^n\}, \quad (3.3)$$

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 [CGS] 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 constructed to a 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 fully discrete space

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

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.

Now we are ready to introduce the fully discrete scheme for (1.4). For brevity, we set $F(v) := v^3 - v$. The backward Euler-finite element method reads: for each $n = 1, \dots, N$, find $U_h^n \in V_{hk}^n$, such that

$$\begin{aligned} k_n^{-1} (U_h^n - U_h^{n-1}, X) + (\nabla U_h^n, \nabla X) + \epsilon^{-2} (F(U_h^n), X) &= \langle f^n, X \rangle, \\ U_h^0 &= \mathcal{P}_h^0 u^0, \end{aligned} \quad (3.4)$$

for every $X \in V_{hk}^n$; here, $f^n := f(t_n)$ and \mathcal{P}_h^n denoting the orthogonal L_2 -projection operator onto the finite element space V_h^n , i.e. $(\mathcal{P}_h^n v, X) = (v, X)$, for all $X \in V_h^n$.

Furthermore, we introduce the discrete Laplacian operator $\Delta_h^n : V_h^n \rightarrow V_h^n$ defined by $(-\Delta_h^n V, X) = (\nabla V, \nabla X)$, for all $V, X \in V_h^n$. This allows the strong representation of (3.4) in strong form as

$$k_n^{-1} (U_h^n - \mathcal{P}_h^n U_h^{n-1}) - \Delta_h^n U_h^n + \epsilon^{-2} \mathcal{P}_h^n F(U_h^n) = \mathcal{P}_h^n f^n. \quad (3.5)$$

3.2.2 Reconstructions

We now introduce a variant of the elliptic reconstruction [MN03, LM06, GLW21], which will be instrumental in the proof of the residual type *a posteriori* error estimators of elliptic problems in Subsection 3.3.4.

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

$$(\nabla \omega^n, \nabla v) = \langle g_h^n, v \rangle, \quad \text{for all } v \in H_0^1(\Omega), \quad (3.6)$$

where

$$\begin{aligned} g_h^n &:= -\Delta_h^n U_h^n - \epsilon^{-2} (F(U_h^n) - \mathcal{P}_h^n F(U_h^n)) - \mathcal{P}_h^n f^n + f^n \\ &\quad - k_n^{-1} (\mathcal{P}_h^n U_h^{n-1} - U_h^{n-1}); \end{aligned} \quad (3.7)$$

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

$$(\nabla(\omega^n - U_h^n), \nabla X) = 0, \quad \text{for all } X \in V_h^n. \quad (3.8)$$

Indeed, choosing $v = X \in V_h^n$ in (3.6), it yields that

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

Then, using the orthogonality property of L_2 -projection operator, \mathcal{P}_h^n , we obtain (3.8). 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 to use *a posteriori* error bounds for elliptic problems to estimate various norms of $\omega^n - U_h^n$ from above,

$$\|\omega^n - U_h^n\| \leq \mathcal{E}(U_h^n, g_h^n; L_p(\Omega)) \quad (3.9)$$

for each $n = 1, \dots, N$ and every $p \geq 2$.

Also, we shall use the continuous piecewise linear interpolants in time of the sequences (t_n, U_h^n) and (t_n, ω^n) . More specifically, we have the following definition.

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

$$U_h(t) := \ell_{n-1}(t)U_h^{n-1} + \ell_n(t)U_h^n, \quad (3.10)$$

$$\omega(t) := \ell_{n-1}(t)\omega^{n-1} + \ell_n(t)\omega^n, \quad (3.11)$$

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

Notice that U_h, ω are continuous functions with respect to time. The above definition implies that the time derivative of U_h is the discrete backward difference at t_n , i.e.,

$$U_{h,t}(t) = \frac{U_h^n - U_h^{n-1}}{k_n}. \quad (3.12)$$

3.3 A posteriori error estimates

We begin by splitting the total error as follows:

$$e := u - U_h = \theta - \rho, \quad \text{where } \theta := \omega - U_h, \rho := \omega - u. \quad (3.13)$$

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 (3.1) with a fully computable right-hand side that consists of θ and the problem data. The following lemma states this error equation.

Lemma 3.4 (error equation). On each J_n , $n = 1, \dots, N$ and for all $v \in H_0^1(\Omega)$, we have

$$\begin{aligned} & \langle \rho_t, v \rangle + (\nabla \rho, \nabla v) + \epsilon^{-2} (F(U_h) - F(u), v) \\ &= \langle f^n - f, v \rangle + \langle \theta_t, v \rangle + \epsilon^{-2} (F(U_h) - F(U_h^n), v) + (\nabla(\omega - \omega^n), \nabla v). \end{aligned} \quad (3.14)$$

Proof. The decomposition of ρ along with (3.1) and (3.6) imply that

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

Next, we combine (3.7) and (3.5) to deduce

$$\begin{aligned} & \langle \rho_t, v \rangle + (\nabla \rho, \nabla v) \\ &= -\langle f - f^n, v \rangle + \epsilon^{-2} (F(u), v) + \langle \omega_t, v \rangle + (\nabla(\omega - \omega^n), \nabla v) + \epsilon^{-2} (F(U_h^n), v) \\ &\quad + (-\Delta_h^n U_h^n + \epsilon^{-2} P_h^n F(U_h^n) + P_h^n f^n, v) - k_n (P_h^n U_h^{n-1} - U_h^{n-1}, v) \\ &= -\langle f - f^n, v \rangle + \epsilon^{-2} (F(u), v) + \langle \omega_t, v \rangle + (\nabla(\omega - \omega^n), \nabla v) \\ &\quad - \epsilon^{-2} (F(U_h^n), v) - k_n ((U_h^n - P_h^n U_h^{n-1}) + (P_h^n U_h^{n-1} - U_h^{n-1}), v), \end{aligned}$$

respectively. Adding to both sides the term $\epsilon^{-2} F(U_h)$ and after standard manipulations, the proof is completed. \square

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 (3.14). For brevity, we set

$$\partial X_n := \frac{X_n - X_{n-1}}{k_n} \quad \forall \{X_n\}_{n \in \mathbb{N} \cup \{0\}}. \quad (3.15)$$

Lemma 3.5. On each J_n , $n = 1, \dots, N$, we have

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

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

Proof. From (3.10), (3.11) 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 (3.7) in conjunction with the strong representation (3.5), we obtain

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

A similar representation can be derived for g_h^{n-1} . Combining the above, the result follows. \square

3.3.1 Energy argument

We begin by introducing some notation. We define

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

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

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

where $C_0 := (\tilde{c}^2 + 1)/2$, $C_1 := 9 + 9C_P \tilde{c}^2 + 6^4 11^2 C_P^2 \tilde{c}^4$ and $C_2 := 2 \cdot 3^7 C_P^2 \tilde{c}^4$, with C_P be the constant of the Poincaré inequality (2.8) while \tilde{c} as in (2.3)-(2.5).

Remark 3.6. The terms in \mathcal{L}_1 and the term $\epsilon^{-4} \|F(U_h^n) - F(U_h^{n-1})\|_{L_2(\Omega)}^2$ 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 for $d = 3$) is often referred as the *spatial error estimate*.

A key ingredient in the proof of the following lemma for $d = 2$ and 3 is the non-standard test function ϕ given in (3.17) below. 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 (3.16) in the course of the energy argument. At the same time, this test function is also responsible for the presence of favourable 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 4th power appearing in the error terms and the 2nd power in the respective estimators. This observation leads to a formally better dependence with respect to $1/\epsilon$ in the continuation argument. At the same time, the choice (3.17) results to 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 $1/\epsilon$ either, as we shall see in the discussion below. The latter terms are ‘compatible’ with the norms of the error ρ appearing in (3.16).

Lemma 3.7 ($d = 2$). Let $d = 2$, u the solution of (3.1) and ω as in (3.11). Assume that $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, we have

$$\begin{aligned} & \frac{1}{4} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ & + \int_0^\tau A(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h)\rho, \rho) \right) dt \\ & \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \Theta_2 + C_0(\mathcal{L}_1 + \mathcal{L}_2)) dt \quad (3.16) \\ & + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \alpha(U_h) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & + \frac{1}{4\epsilon^6} \int_0^\tau \left(\beta(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \gamma(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt, \end{aligned}$$

where

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

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

$$\phi(\cdot, t) = \rho(\cdot, t) \left(\int_t^\tau \rho^2(\cdot, s) ds + 1 \right), \quad t \in [0, \tau]. \quad (3.17)$$

The hypothesis $\rho \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ implies that $\phi \in H_0^1(\Omega)$. Setting $v = \phi$ in (3.14), we have

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

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

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} \|\rho\|_{L_2(\Omega)}^2 + \langle \rho_t, \rho \int_t^\tau \rho^2(s) ds \rangle + (\nabla \rho, \rho \int_t^\tau \nabla \rho^2(s) ds) \\ &\quad + \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h) \rho, \rho) + \epsilon^{-2} \|\rho\|_{L_4(\Omega)}^4 + A(t) \\ &= \langle f^n - f, \phi \rangle + \langle \theta_t, \phi \rangle + \epsilon^{-2} (F(U_h) - F(U_h^n), \phi) + (\nabla(\omega - \omega^n), \nabla \phi) \\ &\quad + 3\epsilon^{-2} (\theta^2 U_h, \phi) + 3\epsilon^{-2} (\rho^2 U_h, \phi) - 6\epsilon^{-2} (\theta \rho U_h, \phi) + \epsilon^{-2} (\theta^3, \phi) \quad (3.18) \\ &\quad + 3\epsilon^{-2} (\theta \rho^2, \phi) + \epsilon^{-2} (F'(U_h) \theta, \phi) - \epsilon^{-2} (F'(U_h) \rho, \rho \int_t^\tau \rho^2(s) ds) \\ &=: \sum_{j=1}^{11} I_j. \end{aligned}$$

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

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

Applying Hölder, GNL for $d = 2$, Poincaré and Young inequalities, respectively, it gives

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

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

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

From Lemma 3.5 and working as before, we have

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

where

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

Next, we split I_2 as follows:

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

and, using Hölder, Poincaré and Young inequalities, we deduce

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

and

$$I_2^2 \leq \frac{1}{2} \|\theta_t\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2.$$

Next, we split

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

which can be bounded as follows:

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

and

$$I_5^2 \leq \frac{9}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{2} \|U_h\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^2.$$

In the same spirit, we also have

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

and, thus,

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

and

$$I_7^2 \leq \frac{6}{\epsilon^2} \|\theta\|_{L_2(\Omega)} \|U_h\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \leq \frac{396}{\epsilon^4} \|U_h\|_{L_\infty(\Omega)}^2 \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{44} \|\rho\|_{L_4(\Omega)}^4.$$

Next, we consider the splitting

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

From which we infer the following bounds:

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

and

$$I_{10}^2 \leq \frac{1}{2\epsilon^4} \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{2} \|F'(U_h)\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^2.$$

Next, we set

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

and we further estimate as follows:

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

For I_6 and I_9 , we proceed as follows: we split the terms as

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

and estimate:

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

Finally for the last term on the right-hand side of (3.18), we have

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

Applying the above estimates into (3.18) and integrating with respect to $t \in (0, \tau)$

and using the identities

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

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

The use of the dimension-dependent GNL inequalities (2.3)-(2.5) necessitates certain modifications in the above argument when $d = 3$. For brevity, we shall only provide the new bounds for the terms which are handled differently to the proof of the two-dimensional case from Lemma 3.7. Nonetheless, the advantages persist for the three-dimensional case.

Lemma 3.8 ($d = 3$). Let $d = 3$, u the solution of (3.1) and ω as in (3.11). Assume that $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, we have

$$\begin{aligned} &\frac{1}{8} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ &+ \int_0^\tau A(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h)\rho, \rho) \right) dt \\ &\leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \tilde{\Theta}_2 + \tilde{C}_0(\mathcal{L}_1 + \mathcal{L}_2)) dt \quad (3.19) \\ &+ \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + (\alpha(U_h) + 1) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ &+ \frac{1}{4\epsilon^{10}} \int_0^\tau \left(\tilde{\beta}(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \tilde{\gamma}(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt, \end{aligned}$$

where we denote by

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

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

Proof. Starting from (3.18), 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 3.7 and is, therefore, omitted. We begin by setting $\zeta(\theta, U_h) := \|\theta\|_{L_\infty(\Omega)} + \|U_h\|_{L_\infty(\Omega)}$.

Then, we have

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

using (2.5) for $d = 3$. Similarly, we have

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

Likewise, using completely analogous arguments, we have

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

The estimation of the remaining I_j on the right-hand of (3.18) are completely analogous to the two-dimensional case with the difference that one applies (2.5) for $d = 3$. Collecting all the estimates, we arrive at the desirable result. \square

3.3.2 Spectral estimates and eigenvalue approximations

To ensure polynomial dependence of the resulting estimates on $1/\epsilon$, a widely used idea is to employ *spectral estimates* of the principal eigenvalue of the linearized Allen-Cahn operator:

$$-\lambda(t) := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\|\nabla v\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(u)v, v)}{\|v\|_{L_2(\Omega)}^2}. \quad (3.20)$$

The celebrated works [Che94, MS95, AF93] showed that λ can be bounded independently of ϵ for the case of smooth, evolved interfaces. This idea was used in [FP03] for

the proof of *a priori* and [KNS04, FW05] for *a posteriori* error bounds for finite element methods in various norms with constants depending upon $1/\epsilon$ only in a polynomial fashion. The *a priori* nature of the spectral estimate (3.20) is somewhat at odds, however, with the presence of λ in *a posteriori* error bounds. This difficulty was overcome in [Bar05] by first linearizing about the numerical solution U_h , viz.,

$$-\Lambda(t) := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\|\nabla v\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h(t))v, v)}{\|v\|_{L_2(\Omega)}^2}, \quad (3.21)$$

and by then proving verifiable eigenvalue approximation error bounds.

Indeed, let us omit the time variable t and consider that there exist functions $w \in H_0^1(\Omega)$ such that

$$(\nabla w, \nabla v) + \epsilon^{-2} (F'(U_h)w, v) = -\Lambda(w, v) \quad \forall v \in H_0^1(\Omega). \quad (3.22)$$

Let P_Λ be the L_2 -projection onto the subspace of all functions $w \in H_0^1(\Omega)$ that satisfy (3.22). The lowest order finite element scheme comprises: We assume that we are given $(w_h, \Lambda_h) \in V_h^n \times \mathbb{R}$ with $\|w_h\|_{L_2(\Omega)} = 1$ such that

$$(\nabla w_h, \nabla v_h) + \epsilon^{-2} (F'(U_h)w_h, v_h) = -\Lambda_h(w_h, v_h) \quad \forall v_h \in V_h^n. \quad (3.23)$$

We present the following upper bounds from [BMO11] for the lowest order finite element scheme, upon choosing $k = 1$ into (3.3):

$$V_h^{n,1} = \{\chi \in C(\bar{\Omega}); \chi|_\tau \in \mathbb{P}_1(\tau), \forall \tau \in \mathcal{T}_h^n\}.$$

Proposition 3.9. [BMO11, Proposition 3.5] Let $(w_h, \Lambda_h) \in V_h^{n,1} \times \mathbb{R}$ satisfy (3.23) with $\|w_h\|_{L_2(\Omega)} = 1$ and assume that

$$\|w_h - P_\Lambda w_h\|_{L_2(\Omega)}^2 \leq 1/2. \quad (3.24)$$

For $l = 1, 2$ set

$$\eta_{\Lambda, l}^2 := \sum_{\tau \in \mathcal{T}_h^n} \|h_n^l (\Delta w_h - \epsilon^{-2} F'(U_h)w_h - \Lambda w_h)\|_{L_2(\tau)}^2 + \sum_{e \in \mathcal{S}_h^n} \|h_n^{l-1/2} [\nabla w_h]\|_{L_2(e)}^2.$$

Then, for $l = 1$ there holds that

$$\Lambda - \Lambda_h \leq 2\tilde{C}\eta_{\Lambda, 1} \left((-\Lambda_h)_+ + \epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \right)^{1/2},$$

while for $l = 2$ and when there exists a constant $C_\Delta > 0$ such that $\|D^2 v\|_{L_2(\Omega)} \leq C_\Delta \|\Delta v\|_{L_2(\Omega)}$ for all $v \in H_0^1(\Omega) \cap H^2(\Omega)$, we have

$$\Lambda - \Lambda_h \leq 2\tilde{C}C_\Delta \eta_{\Lambda, 2} \left(C_v + 2\epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \right)^{1/2},$$

where we denote by $C_v := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \left(\|\nabla v\|_{L_2(\Omega)}^2 / \|v\|_{L_2(\Omega)}^2 \right)$ and $\tilde{C} > 0$ be a (h_n, ϵ) -independent.

[BMO11, Bar05] noticed that the saturation assumption (3.24) is difficult to verify in practice. To address this, these works include the following *a priori* estimate in case that the Laplace operator is H^2 -regular in Ω .

Proposition 3.10. [BMO11, Proposition 3.7] Suppose that $(w_h, \Lambda_h) \in V_h^{n,1} \times \mathbb{R}$ satisfy (3.23) and assume that h_n is such that

$$\tilde{C} C_\Delta \left(C_v + 2\epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \right) h_n^2 \leq 1/2.$$

Then, we have

$$0 \leq \Lambda - \Lambda_h \leq 4 \left(1 + C_v + 4\epsilon^{-2} \|F'(U_h)\|_{L_\infty(\Omega)} \right)^2 \tilde{C} C_\Delta h_n^2.$$

The latter ensures that it is possible to compute principle eigenvalue approximations and to obtain a lower bound $-\bar{\Lambda}(t) \leq -\Lambda(t)$ through *a posteriori* error estimates. It has been shown in [BMO11, Section 3.2] (see also [Bar05, Section 5]) that for linear conforming finite element spaces, ($\kappa = 1$) it is possible to construct $-\bar{\Lambda}(t) \leq -\Lambda(t)$ for almost all $t \in (0, T]$ upon assuming that $\|U_h\|_{L_\infty(\Omega)}$ remains bounded independently of $1/\epsilon$. In Chapter 4, we shall extend the above results to the hp -version FEM setting.

The ϵ -independence λ , (resp. $\Lambda, \bar{\Lambda}$) 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 evolve interfaces past topological changes. To address this, in [BMO11] (see, also [Bar16, BM11]) a crucial observation on the temporal integrability of λ under topological changes was given: during topological changes we have $\lambda(t) \sim 1/\epsilon^2$, but *only* for time periods of length ϵ^2 . Therefore, it has been postulated that there exists an $m > 0$, such that

$$\int_0^T (\lambda(t))_+ dt \leq C + \log(\epsilon^{-m}) \quad (3.25)$$

holds for some constant $C > 0$ *independent* of ϵ , with $\nu_+ := \max\{\nu, 0\}$; notice that for $m = 0$, we return to the earlier case of no topological changes. A number of numerically validated scenarios justifying (3.25) for the scalar Allen-Cahn and its vectorial counterpart, the Ginzburg-Landau equation, can be found in [BMO11]. Moreover, a construction for a $\bar{\Lambda} \in L_1(0, T)$ such that

$$\int_0^T (\bar{\Lambda}(t))_+ dt \geq \int_0^T (\Lambda(t))_+ dt, \quad (3.26)$$

has been provided in [BMO11, Proposition 3.8]. The above motivate the following assumption on the behaviour of the principal eigenvalue Λ , which we shall henceforth adopt.

Assumption 3.11. 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 $-\bar{\Lambda}(t) \leq -\Lambda(t)$ which is *independent* of ϵ .
- (II) There exists an $m > 0$, such that $\int_0^T \Lambda(t) dt \leq C + \log(\epsilon^{-m})$ for some constant $C > 0$ *independent* of ϵ and we can construct a $\bar{\Lambda} \in L_1(0, T)$ such that (3.26) holds.

Remark 3.12. Of course, Assumption 3.11(I) is a special case of Assumption 3.11(II), arising when $m = 0$. Nonetheless, when Assumption 3.11(I) is valid, the resulting *a posteriori* error estimates will have more favourable dependence on the final time T than the estimates that are possible under the more general Assumption 3.11(II).

We shall prove *a posteriori* error estimates under the more general Assumption 3.11(II), commenting, nevertheless, on the differences that would arise in the proof under 3.11(I) instead.

3.3.3 Continuation argument

We begin by noting that, compared to the state-of-the-art estimates of [BMO11, BM11], there are three additional terms on the right hand side of (3.16), (3.19), due to the use of the special test function (3.17): $\|\theta\|_{L_4(0,T;L_4(\Omega))}$ 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 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 in dropping the $\int_0^\tau A(t) dt \geq 0$ terms from the left-hand side of (3.16) and (3.19) for $d = 2$ and $d = 3$, respectively, in the analysis below.

Assuming that the lower bound $-\bar{\Lambda}(t) \leq -\Lambda(t)$ of the principal eigenvalue is available, we set $v = \rho \in H_0^1(\Omega)$ in (3.21), to deduce

$$\begin{aligned} & \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h)\rho, \rho) \\ &= (1 - \epsilon^2) \left(\|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h)\rho, \rho) \right) \\ &\quad + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U_h)\rho, \rho) \\ &\geq -\bar{\Lambda}(t)(1 - \epsilon^2) \|\rho\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U_h)\rho, \rho). \end{aligned} \tag{3.27}$$

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

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

$\mathcal{D}_2 := \max\{4, \alpha(U_h) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 2\}$, and $\mathcal{B}_2 := \max\{16\beta(\theta, U_h), \gamma(\theta, U_h)\}$, we use (3.27) on the left-hand side of (3.16), we note that $-F'(U_h) \leq 1$, and drop $\int_0^\tau A(t) dt$, 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 $E_2 := \exp\left(\int_0^T \mathcal{D}_2(t) dt\right)$ 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

$$I_2 := \left\{ \tau \in [0, T] : \mathcal{N}_{[0, \tau], 2}(\rho) \leq 4\eta_2^4 E_2 \right\}.$$

The set I_2 is non-empty because $0 \in I_2$ and the left-hand side depends continuously on τ . We set $\tau^* := \max I_2$, and we assume that $\tau^* < T$; we aim to arrive at a contradiction. Hence, using the definition of the set 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

$$\eta_2^4 \leq \epsilon^6 (16\bar{\mathcal{B}}_2(T+1)E_2^2)^{-1}, \quad (3.28)$$

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

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

Gronwall'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 $I_2 = [0, T]$.

Likewise, for $d = 3$, we insert the spectral estimate (3.27) into (3.19), and we work as for $d = 2$. Setting

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

$\mathcal{D}_3 := \max\{4, \alpha(U_h) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 3\}$, $\mathcal{B}_3 := \max\{16\tilde{\beta}(\theta, U_h), \tilde{\gamma}(\theta, U_h)\}$, and $\bar{\mathcal{B}}_3 := \sup_{t \in [0, T]} \mathcal{B}_3(t)$, $E_3 := \exp\left(\int_0^T \mathcal{D}_3(t) dt\right)$ through the same argumentation,

we conclude that now the set $I_3 := \{\tau \in [0, T] : \mathcal{N}_{[0, \tau], 3}(\rho) \leq 4\eta_3^4 E_3\}$ equals to $[0, T]$ upon assuming the condition

$$\eta_3^4 \leq \epsilon^{10} (16\bar{\mathcal{B}}_3(T+1)E_3^2)^{-1}. \quad (3.29)$$

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

Lemma 3.13. Assume that (3.28) holds when $d = 2$ or (3.29) holds when $d = 3$. Then, we have the bound

$$\mathcal{N}_{[0, T], d}(\rho) \leq 4\eta_d^4 E_d. \quad (3.30)$$

3.3.4 Fully computable upper bounds

The bound in Lemma 3.13 is still not fully computable, due to various terms involving θ , θ_t and $\rho(0)$, which we shall now further estimate by computable quantities. For the terms involving $\rho(0)$, we have

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

The Sobolev norms of θ appearing on η_d can be further estimated by *a posteriori* bounds for elliptic problems; see, e.g., [Ver96, AO00] for $p = 2$, and [Noc95, DDP00, DG12] for $p = \infty$. We focus, therefore, in the derivation of 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 following dual problem:

$$\begin{cases} -\Delta z = \psi^{p-1} & \text{in } \Omega, \\ z = 0 & \text{on } \partial\Omega; \end{cases} \quad (3.31)$$

on a convex domain, $\Omega \subset \mathbb{R}^d$ for $d \in \{2, 3\}$. Then, there exists a constant $C_\Omega > 0$, depending on the domain Ω , such that

$$\|z\|_{W^{2,p/(p-1)}(\Omega)} \leq C_\Omega \|\psi^{p-1}\|_{L_{p/(p-1)}(\Omega)} = C_\Omega \|\psi\|_{L_p(\Omega)}^{p-1}, \quad \text{for } p \geq 2; \quad (3.32)$$

we refer to [Gri11] for details.

Spatial error estimates. We estimate Θ_2 by residual-type estimators due to the presence of non-Hilbertian norms. In view of Remark 3.2 above, for every $1 \leq n \leq N$ the term

$$\theta^n = w^n - U_h^n$$

is the error of the elliptic problem (3.6), 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 (3.10) and (3.11) 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

$$\begin{aligned} & \sum_{n=1}^N \int_{J_n} \|\theta\|_{L_p(\Omega)}^p dt \\ & \leq \hat{c} \sum_{n=1}^N k_n (\mathcal{E}^p(U_h^n, g_h^n; L_p(\Omega)) + \mathcal{E}^p(U_h^{n-1}, g_h^{n-1}; L_p(\Omega))), \end{aligned} \quad (3.33)$$

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 (3.31) and we have

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

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 [SZ90, AM17], reading: for all $\tau \in \mathcal{T}_h^n$ and $e \in \mathcal{S}_h^n$ it holds that

$$\begin{aligned} \|z - \mathcal{I}_h^n z\|_{L_p(\tau)} &\leq C_{SZ} h_n^l \|z\|_{W^{l,p}(\omega(\tau))}, \\ \|z - \mathcal{I}_h^n z\|_{L_p(e)} &\leq C_{SZ} h_n^{l-1/p} \|z\|_{W^{l,p}(\omega(e))}, \end{aligned} \quad (3.34)$$

for all $l \leq \kappa + 1$ and for some constant $C_{SZ} > 0$ independent of h_n and of the functions involved, denoting by $\omega(e)$ the neighbourhood of elements sharing the face e , and by $\omega(\tau)$ the neighbourhood of elements sharing a whole edge (/face) or a vertex. Continuing in standard fashion, we have

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

using the approximation properties (3.34) of \mathcal{I}_h^n , Then, the elliptic regularity estimate (3.32) implies that

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

$[\![\nabla U_h^n]\!]$ denotes the *jump* across the internal edge e whereby $r_n := g_h^n + \Delta U_h^n$ the *element residual* of the elliptic problem (3.6) at time t_n . The latter turns out to be the residual of the numerical scheme (3.4) also. Indeed, using the (3.5) and (3.7) we obtain that

$$r_n = g_h^n + \Delta U_h^n = -k_n^{-1} (U_h^n - U_h^{n-1}) - \epsilon^{-2} F(U_h^n) + f^n + \Delta U_h^n.$$

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

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

with $\ell_{h,d} = (\ln(1/h_n))^{\alpha_d}$, where $\alpha_2 = 2$ and $\alpha_3 = 1$; we refer to [DG12, Theorem 6.1] and [DK15] for details.

Mesh change estimates. The use of time extensions in (3.10), (3.11) and (3.12) results in decomposing θ_t as follows

$$\theta_t = \omega_t - U_{h,t} = \frac{\omega^n - \omega^{n-1}}{k_n} - \frac{U_h^n - U_h^{n-1}}{k_n}, \quad \text{for each } n = 1, \dots, N, \quad (3.35)$$

where $U_h^n \in V_h^n$ and $U_h^{n-1} \in V_h^{n-1}$ with $V_h^n \neq V_h^{n-1}$ in general. Since the triangulations \mathcal{T}_h^n and \mathcal{T}_h^{n-1} can be different when adaptive mesh refinements take place, we consider 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* of \mathcal{T}_h^n and \mathcal{T}_h^{n-1} , $\check{\mathcal{T}}_h^n := \mathcal{T}_h^n \wedge \mathcal{T}_h^{n-1}$. The latter allows 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 $e \in \check{\mathcal{S}}_h^n \setminus \hat{\mathcal{S}}_h^n$ and $1 \leq p < \infty$ it holds that

$$\|z - \hat{\mathcal{I}}_h^n z\|_{L_p(e)} \leq C_{SZ} (\max_{\omega(e)} \hat{h}_n)^{l-1/p} \|z\|_{W^{l,p}(\omega(e))} \quad \forall l \leq \kappa + 1, \quad (3.36)$$

where $\hat{h}_n := \max(h_n, h_{n-1})$, with $\omega(e)$ denoting the neighbourhood of elements sharing the face e , where, as before, the positive constant C_{SZ} depends only on the shape regularity of the triangulation; here $\check{\mathcal{S}}_h^n$ denotes the interior mesh subordinate to the coarsest common refinement $\check{\mathcal{T}}_h^n := \mathcal{T}_h^n \vee \mathcal{T}_h^{n-1}$ of \mathcal{T}_h^n and \mathcal{T}_h^{n-1} .

Setting $\psi = \theta_t$ on (3.31), we work as before to deduce

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

Standard estimation via Hölder's inequality and (3.36) give, in turn,

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

Finally, the assumed elliptic regularity (3.32), gives the *a posteriori* error estimator

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

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

3.3.5 Main results

Now we are ready to present the main error estimate in the $L_4(0, T; L_4(\Omega))$ -norm.

Theorem 3.14. Let $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ and $f \in L_\infty(0, T; L_4(\Omega))$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. Let u be the solution of (3.1) and U_h is its approximation (3.4). Then, under Assumption (3.11)(II) and the condition

$$\eta_d \leq (16(T+1)\bar{\mathcal{B}}_d E_d^2)^{-1/4} \epsilon^{d-1/2}, \quad (3.37)$$

the following error bound holds

$$\|u - U_h\|_{L_4(0, T; L_4(\Omega))} \leq 2\eta_d ((d-1)E_d)^{1/4} + \|\theta\|_{L_4(0, T; L_4(\Omega))}. \quad (3.38)$$

Proof. Ignoring nonnegative terms on the left-hand side of (3.30), we have

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

the proof follows by a triangle inequality. \square

Remark 3.15. We discuss the regularity of data, i.e., the forcing term f and the initial condition u_0 . It is clear that the above *a posteriori* error analysis depends crucially on the construction of a suitable test function ϕ , (3.17). In order to validate the choice of the test function, it is necessary to enforce the following regularity for the solution: $u \in L_4(0, T; W^{2,4}(\Omega))$ and $u_t \in L_4(0, T; L_4(\Omega))$. This is evident in the analysis through the following hypothesis

$$\rho(t) = u(t) - \omega(t) \in W^{1,4}(\Omega) \quad \text{for a.e. } t \in (0, T],$$

that is imposed in both Lemmas 3.7 and 3.8 and it implies that $\phi \in H_0^1(\Omega)$. The latter allows to test the error equation (4.37) against the test function. Importantly, the enhanced regularity assumptions $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ and $f \in L_\infty(0, T; L_4(\Omega))$ guarantee the desired regularity on u . Furthermore, we note that the regularity concerning the forcing term is imposed indirectly through the elliptic reconstruction estimators in the $L_4(0, T; L_4(\Omega))$ -norm. Indeed, f is a component of the *elemental residual* by construction: for each $n = 1, \dots, N$

$$r_n = k_n^{-1} (U_h^{n-1} - U_h^n) + \Delta U_h^n - \epsilon^{-2} F(U_h^n) + f^n.$$

Remark 3.16. Under the more restrictive Assumption 3.11(I), the continuation argument presented in Section 3.3.3 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 $\bar{\mathcal{D}}_d := \sup_{t \in [0, T]} \max\{4, \alpha(U_h) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + d\}$, $d = 2, 3$, Theorem 3.14 remains valid.

Remark 3.17. We stress that Theorem 3.14 holds also in cases whereby it is *not* possible to assume that $\|U_h\|_{L_\infty(0, T; L_\infty(\Omega))}$ is bounded independently of $1/\epsilon$. We note, however, that $\|U_h\|_{L_\infty(0, T; L_\infty(\Omega))}$ remains uniformly bounded with respect to $1/\epsilon$ 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 3.11.

It is instructive to discuss in detail the dependence of the various terms appearing in (3.37) and (3.38) to assess the practicality of the resulting *a posteriori* error bound above. The computational challenge for $\epsilon \ll 1$ is manifested by the satisfaction of the condition (3.37). Indeed as $\epsilon \rightarrow 0$ the condition (3.37) 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 3.14 for further estimation, which requires (3.37) to be valid.

Assuming 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 was estimated in subsection 3.3.4. 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 3.11(I)), one expects that $E_d \sim 1$ as highlighted in the classical works [Che94, MS95]. When topological changes take place, we can follow [BMO11] and postulate that $E_d \sim \epsilon^{-m}$, $m > 0$. With the above convention, we find that (3.37) becomes

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

for some constant $G_d \geq 1$ and for all $m \geq 0$, thus encapsulating simultaneously both cases of Assumption 3.11.

Hence, the ϵ -dependence for the condition (3.37) appears to be *less* stringent than in the respective conditional *a posteriori* in $L_\infty(0,T;L_2(\Omega))$ - and $L_2(0,T;H^1(\Omega))$ -norms from [Bar05, BMO11, BM11], 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 $L_4(0,T;L_4(\Omega))$ -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.

The new *a posteriori* error analysis appears to also improve the ϵ -dependence on the condition for $L_2(0,T;H^1(\Omega))$ - and $L_\infty(0,T;L_2(\Omega))$ -norms bounds compared to [FW05, Bar05, BMO11, BM11] in certain cases. Of course, the different method of proof above results to different terms appearing in η_d above compared to the respective conditional *a posteriori* error bounds from [FW05, Bar05, BMO11, BM11]. Therefore, the performance of the proposed estimates above has to be assessed numerically before any conclusive statements can made. In particular, we have the following result.

Proposition 3.18 ($L_2(H^1)$ - and $L_\infty(L_2)$ -norm estimates). With the hypotheses of Theorem 3.14 and, assuming condition (3.37), 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 (3.37) implies

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

If we accept that $\eta_d^2 \sim \tilde{\eta}$ from [Bar05, BMO11, BM11], for the sake of the argument, at least at the level of the conditional estimate, (3.37) gives formally favourable 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 [BMO11, BM11].

CHAPTER 4

DG - IPDG ON POLYTOPIC MESHES

Here, we focus on the derivation of *a posteriori* error estimates for the fully-discrete approximations of the Allen-Cahn equation (1.4) in two and three spatial dimensions of an arbitrary order space-time method comprising discontinuous Galerkin time-stepping method (DG), combined with interior penalty discontinuous Galerkin method (IPDG) in space. As for the spatial domain, it is decomposed into general polytopes while arbitrary number of very small faces are allowed. The key motivation for studying this method is the potential it offers in significant computational complexity reduction by the use of few “large” elements of general shape in regions of the solution being $u \approx \pm 1$, while employing aggressively refined elements in the interface regions to resolve the layers. The regularity of the mesh is assumed in the spirit of [CDG21]. For this method, we prove conditional type *a posteriori* error estimates in the $L_4(0, T; L_4(\Omega))$, $L_2(0, T; H^1(S))$ and $L_\infty(0, T; L_2(\Omega))$ -norms that depend polynomially upon the inverse of the interface length ϵ , where we denote by $\|\cdot\|_{H^1(S)}$ the dG-norm that will be defined below. The derived conditional assumptions exhibit analogous ϵ -dependence to the one simpler fully discrete scheme from Chapter 3. This time, we introduce the idea of a *space-time reconstruction* to split the total error, resulting from the combination of *time reconstruction* as introduced in [MN06] and further studied in [SW10, HW17, GLW21] and a variant of the *elliptic reconstruction* [MN03, LM06] that takes into account the mesh change effect. Analogously to the previous chapter, we apply non-standard energy techniques together with a continuation argument to derive an estimator with terms that can be controlled in an *a posteriori* fashion. Again, it will be of crucial importance the availability of a spectral estimate of the linearized Allen-Cahn operator with respect to the approximate solution of the proposed scheme. The statement of the *a posteriori* error estimate requires a lower bound of the principal eigenvalue; to that end we adopt Assumption 3.11. Additionally, we investigate the eigenvalue problem approximation by an *hp*-finite element method to compute the principal eigenvalue and we derive respective *a posteriori* eigenvalue error estimates.

4.1 Space-time discretization

Let $0 = t_0 < t_1 < \dots < t_N = T$. We consider the partition of the time interval $[0, T]$ into subintervals $J_n := (t_{n-1}, t_n]$ where $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ each time step. Let also $\{\mathcal{T}_h^n\}_{n=0}^N$ be a sequence of subdivisions of the domain Ω into general polygonal ($d = 2$) or polyhedral ($d = 3$) elements τ , that are allowed to be modified on each time step. We define a mesh function $h : \bar{\Omega} \rightarrow \mathbb{R}$ such that $h|_\tau := h_\tau$ where $h_\tau := \text{diam}(\tau)$ denotes the diameter of $\tau \in \mathcal{T}_h^n$. In order to introduce interior penalty discontinuous Galerkin method, we associate to each \mathcal{T}_h^n the element-wise discontinuous polynomial space:

$$S_h^n := \{v_h \in L_2(\Omega); v_h|_\tau \in \mathbb{P}_\kappa(\tau), \forall \tau \in \mathcal{T}_h^n\},$$

with \mathbb{P}_κ denoting the d -variate space of polynomials of degree at most $\kappa \in \mathbb{N}$.

Let $\Gamma^n := \cup_{\tau \in \mathcal{T}_h^n} \partial\tau$ the skeleton of the mesh while the interior of the skeleton is denoted by $\Gamma_{\text{int}}^n := \Gamma^n \setminus \partial\Omega$, so that $\Gamma^n = \partial\Omega \cup \Gamma_{\text{int}}^n$. The mesh skeleton is decomposed into $(d-1)$ -dimensional simplicial faces, shared by at most two elements. These are distinct from elemental interfaces, defined as the simply-connected components of the intersection between the boundaries of two neighbouring elements. Within this setting, hanging nodes/edges are naturally permitted, as an interface between two elements may be multi-faced. We refer to **Figure 3** for an illustration for $d = 2$.

Given τ^+, τ^- two elements sharing a $(d-1)$ -dimensional face $e := \tau^+ \cap \tau^- \subset \Gamma_{\text{int}}^n$ with \mathbf{n}^+ and \mathbf{n}^- be the respective outward normal unit vectors on e . We define the averages and jumps for arbitrary functions, $v : \Omega \rightarrow \mathbb{R}$ and $\mathbf{w} : \Omega \rightarrow \mathbb{R}^d$ over each e as it follows:

$$\begin{aligned} \{v\}|_e &:= \frac{1}{2} (v^+ + v^-), & \{\mathbf{w}\}|_e &:= \frac{1}{2} (\mathbf{w}^+ + \mathbf{w}^-), \\ \llbracket v \rrbracket|_e &:= v^+ \mathbf{n}^+ + v^- \mathbf{n}^-, & \llbracket \mathbf{w} \rrbracket|_e &:= \mathbf{w}^+ \cdot \mathbf{n}^+ + \mathbf{w}^- \cdot \mathbf{n}^-. \end{aligned}$$

where $v^\pm := v|_{e \cap \partial\tau^\pm}$ and $\mathbf{w}^\pm := \mathbf{w}|_{e \cap \partial\tau^\pm}$. If $e \subset \partial\tau \cap \partial\Omega$, we set $\{\mathbf{w}\} := \mathbf{w}^+$ and $\llbracket v \rrbracket := v^+ \mathbf{n}^+$.

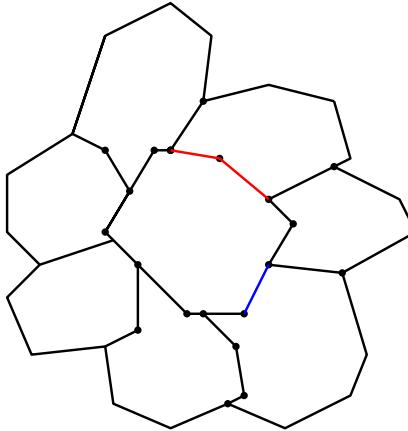


Figure 3: Polygonal element $\tau \in \mathcal{T}_h^n$, and its face-wise neighbours; hanging nodes are highlighted with bold dots, interface and face with red and blue color, respectively.

A finite element space S_h^n is specified on each time interval J_n , $n = 1, \dots, N$. Then, we seek approximate solutions from the space

$$S_{hk} := \left\{ V : (0, T] \rightarrow L_2(\Omega); V|_{J_n} \in \mathbb{P}_{q_n}(J_n; S_h^n) \text{ for each } n = 1, \dots, N \right\},$$

where $\mathbb{P}_{q_n}(J_n; S_h^n)$ denoting the space of polynomials on J_n of degree at most $q_n \in \mathbb{N}_0$, having values in S_h^n . These functions are left continuous with right limits and hence we subsequently write X_n^+ for $X(t_n^-) = X(t_n^-)$ and X_n^+ for $X(t_n^+)$. The jump at t_n will be denoted by $[X]_n = X_n^+ - X_n^-$.

4.1.1 Mesh regularity, inverse estimates and approximation results.

We adopt mesh regularity assumptions in the spirit of [CDG21]. However, in the present context of *a posteriori* error analysis, we require a generalized concept of shape-regularity of the polytopic elements. As such the mesh assumptions presented below are more stringent than the ones in [CDG21]. These assumptions correspond to the dG-norm *a posteriori* error estimates from [CDGon].

Assumption 4.1 (Mesh regularity). Each element $\tau \in \mathcal{T}_h^n$ is a finite union of star-shaped polytopes. Further, there exists a subdivision of each τ into finite non-overlapping polytopes $\{\tau_i\}_{i=1}^{n_\tau}$, that are star shaped with respect to a point $\mathbf{x}_i^* \in \tau_i$ such that

$$C_{sh} \mathbf{m}_i(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \geq h_\tau, \quad (4.1)$$

where $\mathbf{m}_i(\mathbf{x}) := \mathbf{x} - \mathbf{x}_i^*$, $\mathbf{x} \in \partial\tau_i$ and $\mathbf{n}(\mathbf{x})$ the unit outward normal vector to τ_i at $\mathbf{x} \in \partial\tau_i$. Here, $C_{sh} > 1$ is a h_τ -independent constant that holds uniformly through all mesh changes over time steps.

Moreover, there exists $n_e \in \mathbb{N}$ such that for each $\tau \in \mathcal{T}_h^n$ and for each simply connected interface $I \subset \Gamma^n \cap \partial\tau$, it holds that

$$\text{if } C_{sh}|I| \leq h_\tau^{d-1}, \text{ then } \text{card}\{e \in \Gamma^n : e \subset I\} \leq n_e. \quad (4.2)$$

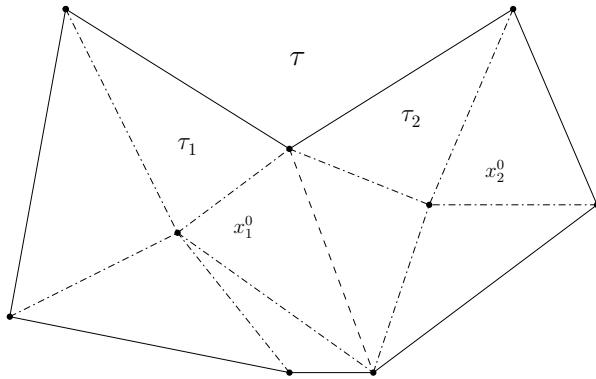


Figure 4: A polygonal element $\tau \in \mathcal{T}_h^n$ with seven nodes is subdivided into two polygons τ_1 and τ_2 star shaped w.r.t. x_1^0 and x_2^0 , respectively.

Lemma 4.2 (Trace estimates [CDG21]). Let $\tau \in T_h^n$ that satisfying Assumption 4.1. Then, for $q \in [1, +\infty)$ and for each $v \in W^{1,q}(\tau)$ the following trace estimate holds for $i = 1, \dots, n_\tau$

$$\begin{aligned} & \|v\|_{L_q(\partial\tau_i)}^q \\ & \leq \frac{d}{\min_{\mathbf{x} \in \partial\tau_i} (\mathbf{m}_i \cdot \mathbf{n})} \|v\|_{L_q(\tau_i)}^q + \frac{q \max_{\mathbf{x} \in \partial\tau_i} |\mathbf{m}_i|_2}{\min_{\mathbf{x} \in \partial\tau_i} (\mathbf{m}_i \cdot \mathbf{n})} \|v\|_{L_q(\tau_i)}^{q-1} \|\nabla v\|_{L_q(\tau_i)}, \end{aligned} \quad (4.3)$$

where $|\cdot|_2$ is the Euclidean distance in \mathbb{R}^d . Moreover, there holds that

$$\|v\|_{L_q(\partial\tau)}^q \leq \sum_{i=1}^{n_\tau} \|v\|_{L_q(\partial\tau_i)}^q \leq C_{\text{tr}} \left(\zeta_1 h_\tau^{-1} \|v\|_{L_p(\tau)}^q + \zeta_2 h_\tau^{q-1} \|\nabla v\|_{L_q(\tau)}^q \right), \quad (4.4)$$

where $C_{\text{tr}} := dC_{\text{sh}}$ and $\zeta_1, \zeta_2 > 0$ algebraic constants that depend on d .

Proof. Applying the Divergence Theorem to the function $|v|^q \mathbf{m}_i$ and verifying that $\nabla \cdot \mathbf{m}_i = d$ it yields that

$$\begin{aligned} \int_{\partial\tau_i} |v|^q \mathbf{m}_i \cdot \mathbf{n} \, ds &= \int_{\tau_i} \nabla \cdot (|v|^q \mathbf{m}_i) \, dx \\ &= \int_{\tau_i} (\nabla \cdot \mathbf{m}_i) |v|^q \, dx + \int_{\tau_i} q|v|^{q-1} |\nabla v| \cdot \mathbf{m}_i \, dx \\ &\leq d \|v\|_{L_q(\tau_i)}^q + q \max_{\mathbf{x} \in \partial\tau_i} |\mathbf{m}_i|_2 \|v\|_{L_q(\tau_i)}^{q-1} \|\nabla v\|_{L_q(\tau_i)}. \end{aligned}$$

Using Hölder, Young inequalities and the property $\max_{\mathbf{x} \in \partial\tau_i} |\mathbf{m}_i|_2 \leq h_\tau$, we derive the second result. \square

We refer to [VV09, Lemma 4.1, Corollary 4.5] for additional details about the construction of a vector field analogous to \mathbf{m}_i defined on simplices and the derivation of the corresponding trace inequalities.

Lemma 4.3 (Inverse estimates [CDG21]). Let $\tau \in T_h^n$ satisfying Assumption 4.1. Then, for $\kappa \in \mathbb{N}$ and for each $v \in \mathbb{P}_\kappa(\tau)$, the following inverse estimate holds

$$\|v\|_{L_2(\partial\tau_i)}^2 \leq \frac{(\kappa+1)(\kappa+d)}{\min_{\mathbf{x} \in \partial\tau_i} (\mathbf{m}_i \cdot \mathbf{n})} \|v\|_{L_2(\tau_i)}^2 \leq C_{\text{sh}} \frac{(\kappa+1)(\kappa+d)}{h_\tau} \|v\|_{L_2(\tau_i)}^2, \quad (4.5)$$

for $i = 1, \dots, n_\tau$. Combining these, we also have

$$\|v\|_{L_2(\partial\tau)}^2 \leq \frac{C_{\text{inv}}}{h_\tau} \|v\|_{L_2(\tau)}^2, \quad (4.6)$$

with C_{inv} a positive constant depending only on κ, d and C_{sh} .

Remark 4.4. Crucially, the constants C_{tr} and C_{inv} do not depend on n_τ , owing to the assumption that the sub-elements τ_i are non-overlapping.

Next, we present the following approximation results.

Lemma 4.5. Let $\tau \in \mathcal{T}_h^n$ satisfying Assumption 4.1. Then, for $q \in [1, +\infty)$ and for all $v \in W^{2,q}(\tau)$ there exists $\Pi_1 v \in \mathbb{P}_1$ such that

$$\|v - \Pi_1 v\|_{L_q(\tau)} \leq C_{\hat{P}}^2 h_\tau^2 |v|_{W^{2,q}(\tau)}, \quad (4.7)$$

$$\|\nabla(v - \Pi_1 v)\|_{L_q(\tau)} \leq C_{\hat{P}} h_\tau |v|_{W^{2,q}(\tau)}, \quad (4.8)$$

with $C_{\hat{P}}$, positive constant depending on d , n_τ and C_{sh} .

Proof. Under the mesh-regularity Assumption 4.1 for $\tau \in \mathcal{T}_h^n$ we can follow the proof of [Ver99, Lemma 4.4] and apply the Poincaré inequalities proved in [VV11, Proposition 2.10] with explicit dependence on the regularity constant C_{sh} , the number of the elemental subdivision n_τ and dimension d . Indeed, we begin by considering the following estimate

$$\|v - \Pi_0 v\|_{L_q(\tau)} \leq C_{\hat{P}} h_\tau \|\nabla v\|_{L_q(\tau)}, \quad (4.9)$$

with $\Pi_0 v$ denoting the orthogonal L_2 -projection onto constants, noting that (4.9) follows immediately from Poincaré inequality and the shape regularity of τ . Let $\Pi_1 v = \alpha_0 + \sum_{i=1}^d \alpha_i x_i$ for $d \in \{2, 3\}$, the elementwise linear polynomial. We choose $\alpha_i = \Pi_0 \left(\frac{\partial v}{\partial x_i} \right)$. Then, since $\frac{\partial \Pi_1 v}{\partial x_i} = \Pi_0 \left(\frac{\partial v}{\partial x_i} \right)$ we obtain that

$$\begin{aligned} & \|\nabla(v - \Pi_1 v)\|_{L_q(\tau)} \\ &= \left(\sum_{i=1}^d \left\| \frac{\partial(v - \Pi_1 v)}{\partial x_i} \right\|_{L_q(\tau)}^q \right)^{1/q} = \left(\sum_{i=1}^d \left\| \frac{\partial v}{\partial x_i} - \Pi_0 \left(\frac{\partial v}{\partial x_i} \right) \right\|_{L_q(\tau)}^q \right)^{1/q} \\ &= \|\nabla v - \Pi_0(\nabla v)\|_{L_q(\tau)} \leq C_{\hat{P}} h_\tau |v|_{W^{2,q}(\tau)}; \end{aligned}$$

at the last step we used the approximation result (4.9). For the proof of (4.7) we set $w = v - \sum_{i=1}^d \alpha_i x_i = v - \sum_{i=1}^d \Pi_0 \left(\frac{\partial v}{\partial x_i} \right) x_i$. Note that

$$v - \Pi_1 v = v - \alpha_0 - \sum_{i=1}^d \alpha_i x_i = w - \alpha_0 = w - \Pi_0 w.$$

Then, we deduce that

$$\begin{aligned} \|v - \Pi_1 v\|_{L_q(\tau)} &= \|w - \Pi_0 w\|_{L_q(\tau)} \leq C_{\hat{P}} h_\tau \|\nabla w\|_{L_q(\tau)} \\ &= C_{\hat{P}} h_\tau \|\nabla(v - \Pi_0 v)\|_{L_q(\tau)} \leq C_{\hat{P}}^2 h_\tau^2 |v|_{W^{2,q}(\tau)}, \end{aligned}$$

using (4.9) and (4.8). \square

Let also

$$\Pi_{hk} := P_h^n \pi_{q_n} : L_2(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n}(J_n; S_h^n)$$

be the time local fully discrete $L_2(J_n; L_2(\Omega))$ -orthogonal projection satisfying

$$\int_{J_n} (\Pi_{hk} X, V) dt = \int_{J_n} (X, V) dt, \quad \text{for all } V \in \mathbb{P}_{q_n}(J_n; S_h^n),$$

where $\pi_{q_n} : L_2(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n}(J_n; L_2(\Omega))$ with

$$\int_{J_n} (\pi_{q_n} X, V) dt = \int_{J_n} (X, V) dt, \quad \text{for all } V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)),$$

for $n = 1, \dots, N$ and P_h^n is the orthogonal L_2 -projection onto S_h^n .

4.1.2 The fully discrete scheme

For brevity, as before, we set $F(U) = U^3 - U$. The above discussion suggests the following space-time dG-method for the problem (1.4) : find $U \in S_{hk}$ such that

$$U(0) = U(t_0^-) := P_h^0 u_0, \quad (4.10)$$

and for $n = 1, \dots, N$ and for each $V \in \mathbb{P}_{q_n}(J_n; S_h^n)$,

$$\begin{aligned} & \int_{J_n} ((U_t, V) + B_n(U, V) + \epsilon^{-2} (F(U), V)) dt + (\llbracket U \rrbracket_{n-1}, V_{n-1}^+) \\ &= \int_{J_n} (f, V) dt, \end{aligned} \quad (4.11)$$

with $B_n \equiv B_n(t) : S_h^n \times S_h^n \rightarrow \mathbb{R}$ the spatial dG-bilinear form, given by

$$\begin{aligned} B_n(w, v) := & \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla w \cdot \nabla v \, dx \\ & - \int_{\Gamma^n} (\{\nabla w\} \cdot \llbracket v \rrbracket + \{\nabla v\} \cdot \llbracket w \rrbracket - \sigma \llbracket w \rrbracket \cdot \llbracket v \rrbracket) \, ds. \end{aligned} \quad (4.12)$$

The nonnegative function $\sigma : \Gamma \rightarrow \mathbb{R}$ is referred to as *discontinuity-penalization parameter*. For the purposes of the error analysis, it is desired the bilinear to be applied to the exact solution u . Thus, we introduce an extension of (4.12) from $S_h^n \times S_h^n$ to $S^n \times S^n$, where $S^n := H_0^1 + S_h^n$, defined by

$$\begin{aligned} \tilde{B}_n(w, v) = & \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla w \cdot \nabla v \, dx \\ & - \int_{\Gamma^n} (\{\mathbf{P}_h^n \nabla w\} \cdot \llbracket v \rrbracket + \{\mathbf{P}_h^n \nabla v\} \cdot \llbracket w \rrbracket - \sigma \llbracket w \rrbracket \cdot \llbracket v \rrbracket) \, ds. \end{aligned} \quad (4.13)$$

Here, $\mathbf{P}_h^n : [L_2(\Omega)]^d \rightarrow [S_h^n]^d$ is the orthogonal L_2 -projection onto the vectorial finite element space. This way, the integrals involving $\{\mathbf{P}_h^n \nabla w\}$ and $\{\mathbf{P}_h^n \nabla v\}$ are well defined as these terms are now traces of element-wise polynomial functions from the finite element space. Furthermore, $A_n : S_h^n \rightarrow S_h^n$ is the discrete dG-Laplacian operator defined by

$$(A_n w, v) = B_n(w, v) = \tilde{B}_n(w, v) \quad \text{for all } w, v \in S_h^n.$$

Note that if $w, v \in H_0^1(\Omega)$, then $\tilde{B}_n(w, v) = (\nabla w, \nabla v)$.

Upon inserting the exact solution u into (4.13) we obtain for every $w \in S^n$ and for each $n = 1, \dots, N$ that

$$\int_{J_n} ((u_t + \epsilon^{-2} F(u) - f, w) + \tilde{B}_n(u, w)) dt = 0,$$

since $\llbracket u \rrbracket_{n-1} = 0$. Integration by parts elementwise with respect to space and the fact that $\llbracket u \rrbracket = 0$ on Γ^n imply that

$$\int_{J_n} (u_t - \Delta u + \epsilon^{-2} F(u) - f, w) dt = \int_{J_n} \int_{\Gamma^n} \{\nabla u - \mathbf{P}_h^n \nabla u\} \cdot \llbracket w \rrbracket \, ds \, dt;$$

the right-hand side is a representation of the inconsistency of $\tilde{B}_n(\cdot, \cdot)$.

Remark 4.6. We denote by $S := S_h + H_0^1(\Omega)$, which can be specified over each time subinterval $J_n, n = 1, \dots, N$ and we write $S^n := S_h^n + H_0^1(\Omega)$.

Now, we assess that the spatial dG-bilinear form (4.13) is symmetric and under a suitable choice of parameter σ it is also coercive. To do so we introduce, the so called dG-norm: for all $w \in S^n$

$$\|w\|_{H^1(S^n)} := \left(\sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} |\nabla w|^2 dx + \int_{\Gamma^n} \sigma |[w]|^2 ds \right)^{1/2}. \quad (4.14)$$

Lemma 4.7. Suppose that $\tau \in \mathcal{T}_h^n$ satisfies Assumption 4.1 for $d \in \{2, 3\}$ and for each $n = 1, \dots, N$. Let also $\sigma := C_{\sigma}(\kappa + 1)(\kappa + d)/h_{\tau}$, where $C_{\sigma} \geq 2C_{sh}$. Then, we have

$$\tilde{B}_n(w, v) \leq \|w\|_{H^1(S^n)} \|v\|_{H^1(S^n)}, \quad \text{for all } w, v \in S^n, \quad (4.15)$$

$$\tilde{B}_n(w, w) \geq \frac{1}{2} \|w\|_{H^1(S^n)}^2, \quad \text{for all } w \in S^n. \quad (4.16)$$

Proof. We begin with the proof of coercivity property. For $w = v$ in (4.13), it yields that

$$\tilde{B}_n(w, w) = \|w\|_{H^1(S^n)}^2 - 2 \int_{\Gamma^n} \{P_h^n \nabla w\} \cdot [w] ds, \quad (4.17)$$

where the last term on the right-hand side can be bounded from above:

$$\begin{aligned} 2 \int_{\Gamma^n} \{P_h^n \nabla w\} \cdot [w] ds &= 2 \int_{\Gamma^n} \sigma^{-1/2} \{P_h^n \nabla w\} \cdot \sigma^{1/2} [w] ds \\ &\leq 2 \int_{\Gamma^n} \sigma^{-1} |\{P_h^n \nabla w\}|^2 ds + \frac{1}{2} \int_{\Gamma^n} \sigma [w]^2 ds. \end{aligned} \quad (4.18)$$

Note that $(P_h^n \nabla w)|_{\tau} \in \mathbb{P}_{\kappa}(\tau), \forall \tau \in \mathcal{T}_h^n$. Then, using the inverse estimate (4.6) where $\kappa \in \mathbb{N}$ and $d \in \{2, 3\}$, we obtain that

$$\begin{aligned} 2 \int_{\Gamma^n} \sigma^{-1} |\{P_h^n \nabla w\}|^2 ds &\leq \sum_{\tau \in \mathcal{T}_h^n} \int_{\partial \tau} \sigma^{-1} |P_h^n \nabla w|^2 ds \\ &\leq \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} C_{sh} \frac{(\kappa + 1)(\kappa + d)}{\sigma h_{\tau}} |P_h^n \nabla w|^2 dx \\ &\leq \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} C_{sh} \frac{(\kappa + 1)(\kappa + d)}{\sigma h_{\tau}} |\nabla w|^2 dx. \end{aligned}$$

At the last step we have used the stability property of the L_2 -projection operator in the L_2 -norm. Then, we choose $C_{\sigma} \geq 2C_{sh}$ and it implies that $C_{sh}(\kappa + 1)(\kappa + d)/\sigma h_{\tau} \leq 1/2$. Thus, inserting the last bound into (4.18) and combining with (4.17), it yields (4.16). For the proof of (4.15) we begin by applying Cauchy-Schwarz inequality and working as before. \square

4.2 Reconstructions

We shall present the main technical tools that will be used throughout the remaining of this chapter. To begin with, we introduce the novel idea of a higher order *time*

reconstruction in the weak sense. Furthermore, we present two different explicit representations based on the original approach of [MN06] and the later works [SW10, HW17]. The next step is the definition of a variant of the *elliptic reconstruction* and its later association with the *time reconstruction* which will be crucial for the proof of the *a posteriori* error bounds below.

4.2.1 Time reconstruction

Let the following time-semidiscrete space

$$S_k := \left\{ V : (0, T] \rightarrow L_2(\Omega); V|_{J_n} \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)), n = 1, \dots, N \right\}. \quad (4.19)$$

We consider the *time reconstruction* $\widehat{W} := R(W)$ where $R : \mathbb{P}_{q_n}(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n+1}(J_n; L_2(\Omega))$ is the so called *reconstruction operator*.

Definition 4.8 (time reconstruction). For $n = 1, \dots, N$, over each time interval J_n we define the *time reconstruction* $\widehat{W}|_{J_n} \in \mathbb{P}_{q_n+1}(J_n; L_2(\Omega))$ of a given time-discrete function $W \in S_k$ such that satisfies for all $V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega))$, $n = 1, \dots, N$,

$$\begin{aligned} \int_{J_n} (\widehat{W}_t, V) dt &= ([W]_{n-1}, V(t_{n-1}^+)) + \int_{J_n} (W_t, V) dt, \\ \widehat{W}(t_{n-1}^+) &= W(t_{n-1}^-). \end{aligned} \quad (4.20)$$

In [MN06, Section 2.1], the *time reconstruction* $\widehat{W} = R(W)$ is constructed elementwise (on each J_n) as the interpolant of a given discontinuous function $W \in S_k$ at the Radau points. Indeed, let $\{\widehat{\ell}_{n-1,j}\}_{j=0}^{q_n+1} \subset \mathbb{P}_{q_n+1}$ be the Lagrange polynomials associated with the Radau points $\{t_{n-1,j}\}_{j=0}^{q_n+1}$ ($t_{n-1,0} = t_{n-1}$ and $t_{n-1,q_n+1} = t_n$) in \bar{J}_n , and define

$$R(W)(t)|_{J_n} := \sum_{j=0}^{q_n+1} \widehat{\ell}_{n-1,j}(t) W(t_{n-1,j});$$

then, $R(W)$ defined as above satisfies (4.20). From [MN06, Lemma 2.1], it follows that $\widehat{W} = R(W)$ is well-defined and continuous on $[0, T]$, satisfying $\widehat{W}(t_{n-1,j}) = W(t_{n-1,j})$, for $j = 1, \dots, q_n + 1$. A consequence of the above useful properties is the following representation of the difference:

$$(\widehat{W} - W)(t)|_{J_n} = \widehat{\ell}_{n-1,0}(t) [W]_{n-1} \quad \forall t \in J_n. \quad (4.21)$$

We emphasize that the above *reconstruction operator* R is usually required for the purpose of the analysis and it does not need to be computed in practice. However, as we shall see below, it may be desirable to compute $R(W)$ when dealing with L_q -norms of the reconstruction error for $p \neq 2, \infty$.

Now, we present an alternative representation of the reconstruction error $\widehat{W} - W$ based on [SW10, Section 4.1] and [GLW21, Section 3.3] rewriting the jumps of W in terms of *lifting* operator. To do so, we consider

$$\chi_n : L_2(\Omega) \rightarrow \mathbb{P}_{q_n}(J_n; L_2(\Omega)), \quad n = 1, \dots, N,$$

a linear *time lifting* operator which is defined for each $v \in L_2(\Omega)$ through

$$\int_{J_n} (\chi_n(v), V) dt = (v, V(t_{n-1}^+)) \quad \text{for each } V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)). \quad (4.22)$$

Then, we can obtain the following characterisation for $t \in \bar{J}_n$

$$\widehat{W}(t)|_{J_n} = W(t_{n-1}^-) + \int_{t_{n-1}}^t (W_t(s) + \chi_n([\![W]\!]_{n-1})(s)) ds, \quad (4.23)$$

that is equivalent to (4.20). Furthermore, integrating by parts with respect to time, we deduce the representation formula

$$(\widehat{W} - W)(t)|_{J_n} = \int_{t_{n-1}}^t \chi_n([\![W]\!]_{n-1})(s) ds - [\![W]\!]_{n-1}, \quad t \in \bar{J}_n. \quad (4.24)$$

We denote by $\varkappa_n : J_n \rightarrow \mathbb{R}$ the polynomial of degree q_n , that represents the *time lifting* (4.22), such that for all $t \in J_n$ and $V \in S_k$

$$\chi_n([\![V]\!]_{n-1})(t) = \varkappa_n(t)[\![V]\!]_{n-1}; \quad (4.25)$$

we refer to [HW17] for an explicit form for \varkappa_n .

Remark 4.9 (computability of \varkappa_n). From [SW10, Lemmas 6, 7], $\varkappa_n(t)$ attains its maximum at t_{n-1} . As a result, we may expect that we can compute $\|\varkappa_n\|_{L_\infty(J_n)} = \frac{q_n+1}{\sqrt{k_n}}$, see [SW10, Proposition 2].

Remark 4.10. The above construction holds also when $q_n = 0$ and it implies that

$$\widehat{W}(t) = W(t_{n-1}^-) + \frac{t - t_{n-1}}{k_n} (W(t_n^-) - W(t_{n-1}^-)) \quad \text{for } t \in \bar{J}_n,$$

which further implies that

$$\widehat{W}_t(t) = \frac{W(t_n^-) - W(t_{n-1}^-)}{k_n}.$$

4.2.2 Elliptic reconstruction

Let $U \in S_{hk}$ be the approximate solution of the fully discrete scheme (4.11) and \widehat{U} the corresponding *time reconstruction* specified on each time subinterval. Now, recalling the above notation we are ready to introduce the *elliptic reconstruction*.

Definition 4.11 (elliptic reconstruction). For each time $t \in J_n$, $n = 1, \dots, N$, we define the elliptic reconstruction $\widetilde{U}(t) \in H_0^1(\Omega)$ by

$$(\nabla \widetilde{U}(t), \nabla v) = (g^n(t), v), \quad \text{for all } v \in H_0^1(\Omega) \quad (4.26)$$

with initial value $\widetilde{U}(0) = \widetilde{U}(t_0^-) := u_0$ and

$$\begin{aligned} g^n(t) := & A_n U(t) - \Pi_{hk} f(t) + \pi_{q_n} f(t) - \epsilon^{-2} \left(\pi_{q_n} F(U(t)) - \Pi_{hk} F(U(t)) \right) \\ & + P_h^n \widehat{U}_t(t) - \widehat{U}_t(t). \end{aligned} \quad (4.27)$$

Remark 4.12 (mesh change indicator). The expression $P_h^n \widehat{U}_t - \widehat{U}_t$, which appears in the definition of *elliptic reconstruction* (4.27), is referred to as the *mesh change indicator*. Indeed, on each J_n ,

$$\begin{aligned} P_h^n \widehat{U}_t - \widehat{U}_t &= P_h^n (U_t + \chi_n ([\![U]\!]_{n-1})) - (U_t + \chi_n ([\![U]\!]_{n-1})) \\ &= \chi_n (P_h^n ([\![U]\!]_{n-1}) - [\![U]\!]_{n-1}) = \chi_n (U_{n-1}^- - P_h^n U_{n-1}^-). \end{aligned}$$

Then, from (4.25), we get

$$P_h^n \widehat{U}_t - \widehat{U}_t = \varkappa_n(t) (U_{n-1}^- - P_h^n U_{n-1}^-), \quad t \in J_n, \quad (4.28)$$

where $U_{n-1}^- \in S_h^{n-1}$ and $P_h^n U_{n-1}^- \in S_h^n$.

Remark 4.13 (properties of the elliptic reconstruction). From (4.26) and (4.27), it follows that since $\tilde{U} \in S_k$ can be written, for any $n = 1, \dots, N$

$$-\Delta \tilde{U}(t) = g^n(t) \quad \text{for each } t \in J_n. \quad (4.29)$$

Moreover, for each $t \in J_n$, $n = 1, \dots, N$, the fully discrete solution $U(t)$ is also the spatial dG-solution to the elliptic problem (4.26). Indeed, let $\tilde{U}_h \in S_h^n$ be the spatial dG-approximation to \tilde{U} , defined for all $V_h \in S_h^n$ by

$$\begin{aligned} B_n(\tilde{U}_h, V_h) &= (g^n, V_h) \\ &= (A_n U, V_h) + (\pi_{q_n} f - P_h^n \pi_{q_n} f, V_h) + (P_h^n \widehat{U}_t - \widehat{U}_t, V_h) \\ &\quad + \epsilon^{-2} (P_h^n \pi_{q_n} F(U) - \pi_{q_n} F(U), V_h). \end{aligned}$$

Then, due to the orthogonality property of the L_2 -projection into S_h^n and the definition of dG-Laplacian operator, it yields that

$$B_n(\tilde{U}_h, V_h) = (A_n U, V_h) = B_n(U, V_h) \quad \text{for all } V_h \in S_h^n, \quad (4.30)$$

which implies that $U = \tilde{U}_h$. This observation, allow us derive *a posteriori* estimators of the *elliptic reconstruction* error

$$\|\tilde{U}(t) - U(t)\|_{L_p(\Omega)} \leq \mathcal{E}(U(t), g^n(t); L_p(\Omega)) \quad \text{for all } t \in J_n. \quad (4.31)$$

A difficulty arises from the lack of the orthogonality of the *elliptic reconstruction* error into the space S_h^n , which is a useful property in the derivation of *a posteriori* error analysis of elliptic problems. This is consequence of the inconsistency of the spatial dG-bilinear form, $\tilde{B}_n(\cdot, \cdot)$, with respect to the elliptic problem (3.6). We overcome this difficulty by introducing ‘something like orthogonality’ in the following lemma.

Lemma 4.14. For all $V_h \in S_h^n$, we have

$$\tilde{B}_n(\tilde{U} - U, V_h) = \int_{\Gamma^n} \{\nabla \tilde{U} - \mathbf{P}_h^n \nabla \tilde{U}\} \cdot [\![V_h]\!] \, ds. \quad (4.32)$$

Proof. From the definition of the extended dG-bilinear form (4.13), we have

$$\begin{aligned}\tilde{B}_n(\tilde{U} - U, V_h) &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla(\tilde{U} - U) \cdot \nabla V_h \, dx - \int_{\Gamma^n} \{\mathbf{P}_h^n \nabla(\tilde{U} - U)\} \cdot [\![V_h]\!] \, ds \\ &\quad - \int_{\Gamma^n} (\{\mathbf{P}_h^n \nabla V_h\} \cdot [\![\tilde{U} - U]\!] - \sigma [\![V_h]\!] \cdot [\![\tilde{U} - U]\!]) \, ds \\ &= -\tilde{B}_n(U, V_h) + \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla \tilde{U} \cdot \nabla V_h \, dx - \int_{\Gamma^n} \{\mathbf{P}_h^n \nabla \tilde{U}\} \cdot [\![V_h]\!] \, ds \\ &\quad - \int_{\Gamma^n} (\{\nabla V_h\} \cdot [\![\tilde{U}]\!] - \sigma [\![V_h]\!] \cdot [\![\tilde{U}]\!]) \, ds.\end{aligned}$$

Note that $[\![\tilde{U}]\!] = 0$ on Γ^n , due to the elliptic regularity on Γ_{int}^n and due to the boundary condition on $\partial\Omega$. According to (4.30), it holds that $\tilde{B}_n(U, V_h) = B_n(U, V_h) = (g^n, V_h)$. The Green's formula implies that

$$\tilde{B}_n(\tilde{U} - U, V_h) = -(g^n, V_h) - \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \Delta \tilde{U} V_h \, dx + \int_{\Gamma} \{\nabla \tilde{U} - \mathbf{P}_h^n \nabla \tilde{U}\} \cdot [\![V_h]\!] \, ds.$$

Finally, along with relation (4.29), we arrive at the desirable result. \square

Note that the *time reconstruction* of the dG-solution U of (4.11) allows the dG space-time formulation to be rewritten in strong form. Furthermore, it enables the direct association of *time reconstruction* with *elliptic reconstruction* that is necessary later for application of the energy argument.

Indeed, let $V \in S_{hk}$. Using the weak definition of *time reconstruction* (4.20), the fully discrete scheme (4.11) becomes

$$\int_{J_n} (\widehat{U}_t + A_n U + \epsilon^{-2} F(U) - f, V) \, dt = 0, \quad n = 1, \dots, N. \quad (4.33)$$

Then, for each $n = 1, \dots, N$, we have that

$$\Pi_{hk} \widehat{U}_t(t) + A_n U(t) + \epsilon^{-2} \Pi_{hk} F(U(t)) - \Pi_{hk} f(t) = 0, \quad \text{for each } t \in J_n.$$

We obtain from (4.24) and (4.25) that for each $t \in J_n$

$$\widehat{U}_t = U_t + \varkappa_n(t) (U_{n-1}^+ - U_{n-1}^-),$$

where $U_{n-1}^+ \in S_h^n$ and $U_{n-1}^- \in S_h^{n-1}$, with $S_h^n \neq S_h^{n-1}$. The latter representation implies that $\widehat{U}_t \in \mathbb{P}_{q_n}(J_n; S_h^n \cup S_h^{n-1})$. As a result it yields that $\Pi_{hk} \widehat{U}_t = \pi_{q_n} P_h^n \widehat{U}_t = P_h^n \widehat{U}_t$. The projections commute i.e., $P_h^n \pi_{q_n} = \pi_{q_n} P_h^n$. Finally, based on the definition of the *elliptic reconstruction*, through (4.26) and (4.27), for each $n = 1, \dots, N$ we may deduce the following pointwise representation

$$\widehat{U}_t(t) - \Delta \tilde{U}(t) + \epsilon^{-2} \pi_{q_n} F(U(t)) = \pi_{q_n} f(t), \quad \text{for each } t \in J_n. \quad (4.34)$$

4.3 A posteriori error estimates

Now we continue by proving *a posteriori* error bounds in the $L_4(0, T; L_4(\Omega))$ -, $L_\infty(0, T; L_2(\Omega))$ - and $L_2(0, T; H^1(S))$ -norms by combining *space-time reconstruction* with continuation arguments and an ‘improved’ spectral estimate regarding the linearized Allen-Cahn operator about the approximate solution U . An important technical difference, compared to the results of Chapter 3, is the lack of availability of $L_\infty(\Omega)$ -norm elliptic *a posteriori* error bounds on polytopic meshes. In Chapter 3, $L_\infty(\Omega)$ -norm *a posteriori* error estimates are used to bound $\|\theta\|_{L_\infty(\Omega)}$ from above. In this chapter, we shall modify the estimates to avoid the presence of $\|\theta\|_{L_\infty(\Omega)}$. Instead, we opt for estimates involving only $\|\theta\|_{L_p(\Omega)}$ for $2 \leq p < +\infty$ and derive *a posteriori* elliptic estimators on polytopic meshes.

Let $\omega := \widehat{\tilde{U}}$ be the *time reconstruction* of the *elliptic reconstruction*, which is valid since $\tilde{U} \in S_k$. We split the total error as in [GLW21]:

$$e := u - U = \theta - \rho, \quad \text{where } \theta := \omega - U, \rho := \omega - u. \quad (4.35)$$

We can alternatively write

$$\theta := \omega - U = (\widehat{\tilde{U}} - \tilde{U}) + (\tilde{U} - U); \quad (4.36)$$

these are referred to as *time reconstruction* error and *space reconstruction* error respectively and can be bounded in various norms by estimators that are explicitly computable; this shall be performed in detail in Section 4.4. Thus, it suffices to estimate ρ in terms of θ and the problem data. To do so, along with relations (3.1) and (4.34) and elementary manipulations lead to the following error equation:

Lemma 4.15 (error relation). On J_n , $n = 1, \dots, N$ and for all $v \in H_0^1(\Omega)$, it holds,

$$\begin{aligned} & (\rho_t, v) + (\nabla \rho, \nabla v) + \epsilon^{-2} (F(U) - F(u), v) \\ &= (\pi_{q_n} f - f, v) + ((\omega - \widehat{U})_t, v) + (\nabla(\omega - \tilde{U}), \nabla v) \\ & \quad + \epsilon^{-2} (F(U) - \pi_{q_n} F(U), v). \end{aligned} \quad (4.37)$$

Norms of ρ will be further estimated through PDE stability arguments below.

Remark 4.16. We prefer to split the total error using the $\widehat{\tilde{U}}$ be the *time reconstruction* of the *elliptic reconstruction* according to [GLW21, Section 5] instead of acting like in [GLW21, Section 4] and considering an error decomposition of the form

$$e := u - U = \hat{e} + \hat{\sigma} = \tilde{e} + \tilde{\sigma},$$

where $\hat{e} := u - \widehat{U}$, $\hat{\sigma} := \widehat{U} - U$ and $\tilde{e} := u - \tilde{U}$, $\tilde{\sigma} := \tilde{U} - U$. The main reason is that the latter leads to an error relation that is not suitable to derive estimates in the $L_4(0, T; L_4(\Omega))$ -norm. Even if we are interested in studying the error only in the $L_2(0, T; H^1(S))$ -norm, we will deduce to more stringent conditions with respect to ϵ -dependence.

4.3.1 Energy argument

We begin by introducing some notation that will use to state the main results. We define on each J_n , $n = 1, \dots, N$,

$$\begin{aligned}\mathcal{L}_1^{\text{dG}}(t) &:= \|\Delta(\omega - \tilde{U})\|_{L_2(\Omega)}^2, \\ \mathcal{L}_2^{\text{dG}}(t) &:= \|\pi_{q_n} f - f\|_{L_2(\Omega)}^2 + \epsilon^{-4} \|F(U) - \pi_{q_n} F(U)\|_{L_2(\Omega)}^2.\end{aligned}$$

Furthermore, we set for brevity

$$\begin{aligned}\Theta_1^{\text{dG}}(t) &:= \frac{1}{2} \|(\omega - \hat{U})_t\|_{L_2(\Omega)}^2 + \frac{3C_P^4}{2} \|(\omega - \hat{U})_t\|_{L_4(\Omega)}^4, \\ \Theta_2^{\text{dG}}(t) &:= \epsilon^{-4} \left((C_0 + 216\|U\|_{L_\infty(\Omega)}^2) \|\theta\|_{L_2(\Omega)}^2 + C_1 \|\theta\|_{L_4(\Omega)}^4 + C_0 \|\theta\|_{L_6(\Omega)}^6 \right), \\ A^{\text{dG}}(t) &:= \epsilon^{-2} \left((\theta^2 \rho^2 + \rho^4 + |\nabla \rho|^2, \int_t^\tau \rho^2(s) ds) + (\theta^2, \rho^2) \right),\end{aligned}$$

with $C_0 := (C_P \tilde{c}^2 + 1)/2$, $C_1 := (9C_P \tilde{c}^2 + 6^6 C_P^2 \tilde{c}^4 + 3^7 2^{-4} \epsilon^2 + 9)/2$, $C_2 := 3^7 C_P^2 \tilde{c}^4 + 3^7 (1 + C_P^2)^2 \tilde{c}^4$. Here, C_P is the constant of the Poincaré inequality $\|v\|_{L_2(\Omega)} \leq C_P \|\nabla v\|_{L_2(\Omega)}$, while \tilde{c} is the embedding constant of $\|v\|_{L_8(\Omega)} \leq \tilde{c} \|v\|_{H^1(\Omega)}$ and \tilde{c} as in (2.3) - (2.5).

Lemma 4.17 ($d = 2$). Let u be the solution of (3.1). Assume that $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, we have

$$\begin{aligned}&\frac{1}{8} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\&+ \int_0^\tau A^{\text{dG}}(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2} \right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U) \rho, \rho) \right) dt \\&\leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1^{\text{dG}} + \Theta_2^{\text{dG}} + C_0 (\mathcal{L}_1^{\text{dG}} + \mathcal{L}_2^{\text{dG}})) dt \quad (4.38) \\&+ \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \alpha^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\&+ \frac{1}{4\epsilon^6} \int_0^\tau \left(\beta^{\text{dG}}(\theta, U) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \gamma^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^4 \right) dt,\end{aligned}$$

where

$$\begin{aligned}\alpha^{\text{dG}}(U) &:= \|F'(U)\|_{L_\infty(\Omega)}^2 + \|U\|_{L_\infty(\Omega)}^2 + 5 \\ \beta^{\text{dG}}(\theta, U) &:= C_2 \epsilon^4 (\|\theta\|_{L_8(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4) + 2\epsilon^2 \|U\|_{L_\infty(\Omega)}^4 \\ &\quad + 2C_P^2 \tilde{c}^4 \|F'(U)\|_{L_\infty(\Omega)}^2 + 6\epsilon^6 (\|F'(U)\|_{L_\infty(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4 + 4), \\ \gamma^{\text{dG}}(U) &:= 2\tilde{c}^4 (C_P^2 \|F'(U)\|_{L_\infty(\Omega)}^2 + 18 \|U\|_{L_\infty(\Omega)}^2).\end{aligned}$$

Proof. Using Taylor's theorem, it yields that

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

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

$$\phi(\cdot, t) = \rho(\cdot, t) \left(\int_t^\tau \rho^2(\cdot, s) ds + 1 \right), \quad t \in [0, \tau]. \quad (4.39)$$

Assumption $\rho \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ implies that $\phi \in H_0^1(\Omega)$. Setting $v = \phi$ in (4.37), we have

$$\begin{aligned} & (\rho_t, \phi) + (\nabla \rho, \nabla \phi) - \epsilon^{-2}(eF'(U) + 3e^2U + e^3, \phi) \\ &= (\pi_{q_n} f - f, \phi) + ((\omega - \widehat{U})_t, \phi) + (\nabla(\omega - \widetilde{U}), \nabla \phi) + \epsilon^{-2}(F(U) - \pi_{q_n} F(U), \phi). \end{aligned}$$

Using now the following identities

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

and after some elementary manipulations, we deduce

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|\rho\|_{L_2(\Omega)}^2 + (\rho_t, \rho \int_t^\tau \rho^2(s) ds) + (\nabla \rho, \rho \int_t^\tau \nabla \rho^2(s) ds) \\ &+ \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2}(F'(U)\rho, \rho) + \epsilon^{-2}\|\rho\|_{L_4(\Omega)}^4 + A^{\text{dG}}(t) \\ &= (\pi_{q_n} f - f, \phi) + ((\omega - \widehat{U})_t, \phi) + (\nabla(\omega - \widetilde{U}), \nabla \phi) \\ &+ \epsilon^{-2}(F(U) - \pi_{q_n} F(U), \phi) + 3\epsilon^{-2}(\theta^2 U, \phi) + 3\epsilon^{-2}(\rho^2 U, \phi) \\ &- 6\epsilon^{-2}(\theta \rho U, \phi) + \epsilon^{-2}(\theta^3, \phi) + 3\epsilon^{-2}(\theta \rho^2, \phi) + \epsilon^{-2}(F'(U)\theta, \phi) \\ &- \epsilon^{-2}(F'(U)\rho, \rho \int_t^\tau \rho^2(s) ds) =: \sum_{j=1}^{11} I_j. \end{aligned} \quad (4.40)$$

We shall estimate each I_j , $j = 1, \dots, 11$. We begin by splitting I_1 ,

$$I_1 = (\pi_{q_n} f - f, \rho \int_t^\tau \rho^2(s) ds) + (\pi_{q_n} f - f, \rho) =: I_1^1 + I_1^2.$$

Applying Hölder, GNL ($d = 2$), Poincaré and Young's inequalities we obtain

$$\begin{aligned} I_1^1 &\leq \|\pi_{q_n} f - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq \tilde{c} \|\pi_{q_n} f - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \\ &\leq C_P^{1/2} \tilde{c} \|\pi_{q_n} f - f\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{C_P \tilde{c}^2}{2} \|\pi_{q_n} f - f\|_{L_2(\Omega)}^2 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \end{aligned}$$

while Cauchy-Schwarz and Young's inequalities imply

$$I_1^2 \leq \frac{1}{2} \|\pi_{q_n} f - f\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2.$$

Similarly we split

$$I_2 = ((\omega - \widehat{U})_t, \rho \int_t^\tau \rho^2(s) ds) + ((\omega - \widehat{U})_t, \rho) =: I_2^1 + I_2^2.$$

Therefore, the resulting terms can be bounded as follows

$$\begin{aligned} I_2^1 &\leq \|(\omega - \widehat{U})_t\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq C_P \|(\omega - \widehat{U})_t\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{3C_P^4}{2} \|(\omega - \widehat{U})_t\|_{L_4(\Omega)}^4 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{1}{2} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2, \\ I_2^2 &\leq \frac{1}{2} \|(\omega - \widehat{U})_t\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

Next, splitting I_3 and using the same inequalities, it yields

$$I_3 = (\nabla(\omega - \widetilde{U}), \nabla(\rho \int_t^\tau \rho^2(s) ds)) + (\nabla(\omega - \widetilde{U}), \nabla\rho) := I_3^1 + I_3^2,$$

with bounds,

$$\begin{aligned} I_3^1 &\leq \frac{C_P \tilde{c}^2}{2} \mathcal{L}_1^{\text{dG}} + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_3^2 &\leq \frac{1}{2} \mathcal{L}_1^{\text{dG}} + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

In the same spirit, we set

$$I_4 = \epsilon^{-2} (F(U) - \pi_{q_n} F(U), \rho \int_t^\tau \rho^2(s) ds) + \epsilon^{-2} (F(U) - \pi_{q_n} F(U), \rho) =: I_4^1 + I_4^2,$$

yielding the following bounds

$$\begin{aligned} I_4^1 &\leq \frac{C_P \tilde{c}^2}{2\epsilon^4} \|F(U) - \pi_{q_n} F(U)\|_{L_2(\Omega)}^2 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_4^2 &\leq \frac{1}{2\epsilon^4} \|F(U) - \pi_{q_n} F(U)\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

Next, we split $I_5 = 3\epsilon^{-2} (\theta^2 U, \rho \int_t^\tau \rho^2(s) ds) + 3\epsilon^{-2} (\theta^2 U, \rho) =: I_5^1 + I_5^2$,

$$\begin{aligned} I_5^1 &\leq 3\epsilon^{-2} \|\theta^2\|_{L_2(\Omega)} \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq 3\epsilon^{-2} \tilde{c} \|\theta\|_{L_4(\Omega)}^2 \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/2} \\ &\leq 3\epsilon^{-2} C_P^{1/2} \tilde{c} \|\theta\|_{L_4(\Omega)}^2 \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{9C_P \tilde{c}^2}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2} \|U\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \end{aligned}$$

and

$$I_5^2 \leq \frac{9}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{2} \|U\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^2.$$

For $I_6 = 3\epsilon^{-2}(\rho^2 U, \rho \int_t^\tau \rho^2(s) ds) + 3\epsilon^{-2}(\rho^2 U, \rho) =: I_6^1 + I_6^2$, we work as follows

$$\begin{aligned} I_6^1 &\leq \frac{3C_P^{1/2}\tilde{c}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \|U\|_{L_\infty(\Omega)} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{4\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{3^7\tilde{c}^4 C_P^2}{4\epsilon^2} \|U\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_6^2 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^2 \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \leq \frac{\epsilon^2}{4} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{9\tilde{c}^4}{\epsilon^6} \|U\|_{L_\infty(\Omega)}^2 \|\rho\|_{L_2(\Omega)}^4. \end{aligned}$$

We also set $I_7 = -6\epsilon^{-2}(\theta \rho U, \rho \int_t^\tau \rho^2(s) ds) - 6\epsilon^{-2}(\theta \rho U, \rho) =: I_7^1 + I_7^2$ and we further obtain that

$$\begin{aligned} I_7^1 &\leq 6\epsilon^{-2} \|\theta\|_{L_4(\Omega)} \|\rho^2\|_{L_2(\Omega)} \|U\|_{L_\infty(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq \frac{6C_P^{1/2}\tilde{c}}{\epsilon^2} \|\theta\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \|U\|_{L_\infty(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{6^6 C_P^2 \tilde{c}^4}{2\epsilon^4} \|\theta\|_{L_4(\Omega)}^4 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{1}{2\epsilon^4} \|U\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_7^2 &\leq \frac{6}{\epsilon^2} \|\theta\|_{L_2(\Omega)} \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_4(\Omega)}^2 \leq \frac{216}{\epsilon^4} \|U\|_{L_\infty(\Omega)}^2 \|\theta\|_{L_2(\Omega)}^2 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4. \end{aligned}$$

Now we consider the splitting $I_8 = \epsilon^{-2}(\theta^3, \rho \int_t^\tau \rho^2(s) ds) + \epsilon^{-2}(\theta^3, \rho) =: I_8^1 + I_8^2$, that allows to estimate

$$\begin{aligned} I_8^1 &\leq \epsilon^{-2} \|\theta^3\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq \frac{C_P^{1/2}\tilde{c}}{\epsilon^2} \|\theta\|_{L_6(\Omega)}^3 \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{C_P \tilde{c}^2}{2\epsilon^4} \|\theta\|_{L_6(\Omega)}^6 + \frac{1}{24} \|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \\ I_8^2 &\leq \frac{1}{2\epsilon^4} \|\theta\|_{L_6(\Omega)}^6 + \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

For $I_9 = 3\epsilon^{-2}(\rho^2\theta, \rho \int_t^\tau \rho^2(s) ds) + 3\epsilon^{-2}(\rho^2\theta, \rho) =: I_9^1 + I_9^2$, we obtain the bounds

$$\begin{aligned} I_9^1 &\leq 3\epsilon^{-2}\|\rho\|_{L_4(\Omega)}^3\|\theta\|_{L_8(\Omega)}\left\|\int_t^\tau \rho^2(s) ds\right\|_{L_8(\Omega)} \\ &\leq 3\hat{c}\epsilon^{-2}\|\rho\|_{L_4(\Omega)}^3\|\theta\|_{L_8(\Omega)}\left\|\int_t^\tau \rho^2(s) ds\right\|_{H^1(\Omega)} \\ &\leq 3\hat{c}(1+C_P^2)^{1/2}\epsilon^{-2}\|\rho\|_{L_4(\Omega)}^3\|\theta\|_{L_8(\Omega)}\left\|\int_t^\tau \nabla \rho^2(s) ds\right\|_{L_2(\Omega)} \\ &\leq \frac{1}{4\epsilon^2}\|\rho\|_{L_4(\Omega)}^4 + \frac{3^7\hat{c}^4(1+C_P^2)^2}{4\epsilon^2}\|\theta\|_{L_8(\Omega)}^4\left\|\int_t^\tau \nabla \rho^2(s) ds\right\|_{L_2(\Omega)}^4, \\ I_9^2 &\leq 3\epsilon^{-2}\|\rho\|_{L_4(\Omega)}^3\|\theta\|_{L_4(\Omega)} \leq \frac{1}{2\epsilon^2}\|\rho\|_{L_4(\Omega)}^4 + \frac{3^7}{25\epsilon^2}\|\theta\|_{L_4(\Omega)}^4. \end{aligned}$$

Next, we set $I_{10} = \epsilon^{-2}(F'(U)\theta, \rho \int_t^\tau \rho^2(s) ds) + \epsilon^{-2}(F'(U)\theta, \rho) =: I_{10}^1 + I_{10}^2$, and we have the following bounds:

$$\begin{aligned} I_{10}^1 &\leq \epsilon^{-2}\|F'(U)\|_{L_\infty(\Omega)}\|\theta\|_{L_2(\Omega)}\|\rho\|_{L_4(\Omega)}\left\|\int_t^\tau \rho^2(s) ds\right\|_{L_4(\Omega)} \\ &\leq \frac{C_P^{1/2}\tilde{c}}{\epsilon^2}\|F'(U)\|_{L_\infty(\Omega)}\|\theta\|_{L_2(\Omega)}\|\rho\|_{L_4(\Omega)}\left\|\int_t^\tau \nabla \rho^2(s) ds\right\|_{L_2(\Omega)} \\ &\leq \frac{C_P\tilde{c}^2}{2\epsilon^4}\|\theta\|_{L_2(\Omega)}^2 + \frac{1}{24}\|\rho\|_{L_4(\Omega)}^4 + \frac{3}{2}\|F'(U)\|_{L_\infty(\Omega)}^4\left\|\int_t^\tau \nabla \rho^2(s) ds\right\|_{L_2(\Omega)}^4, \\ I_{10}^2 &\leq \frac{1}{2\epsilon^4}\|\theta\|_{L_2(\Omega)}^2 + \frac{1}{2}\|F'(U)\|_{L_\infty(\Omega)}^2\|\rho\|_{L_2(\Omega)}^2. \end{aligned}$$

Finally for the last term on the right-hand side of (4.40), we have

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

Inserting the above estimates into (4.40), integrating with respect to $t \in (0, \tau)$ along with elementary manipulation, we arrive at the desirable result. \square

Lemma 4.18 ($d = 3$). Let u be the solution of (3.1). Assume that $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ for a.e. $t \in (0, T]$. Then, for any $\tau \in (0, T]$, it holds that

$$\begin{aligned} & \frac{1}{16} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ & + \int_0^\tau A^{\text{dG}}(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U)\rho, \rho) \right) dt \quad (4.41) \\ & \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1^{\text{dG}} + \tilde{\Theta}_2^{\text{dG}} + \tilde{C}_0(\mathcal{L}_1^{\text{dG}} + \mathcal{L}_2^{\text{dG}})) dt \\ & + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + (\alpha^{\text{dG}}(U) + 1) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & + \frac{1}{4\epsilon^{10}} \int_0^\tau \left(\tilde{\beta}^{\text{dG}}(\theta, U) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \tilde{\gamma}^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^4 \right) dt, \end{aligned}$$

where

$$\begin{aligned} \tilde{\Theta}_2^{\text{dG}}(t) &:= \epsilon^{-4} \left((\tilde{C}_0 + 216 \|U\|_{L_\infty(\Omega)}^2) \|\theta\|_{L_2(\Omega)}^2 + \tilde{C}_1 \|\theta\|_{L_4(\Omega)}^4 + \tilde{C}_0 \|\theta\|_{L_6(\Omega)}^6 \right), \\ \tilde{\beta}^{\text{dG}}(\theta, U) &:= 3^7 \epsilon^8 (\hat{C}^4 \|\theta\|_{L_{12}(\Omega)}^4 + C_P \tilde{c}^4 \|U\|_{L_\infty(\Omega)}^4) + 2\epsilon^6 \|U\|_{L_\infty(\Omega)}^4 \\ &+ 4C_P \tilde{c}^4 \epsilon^2 \|F'(U)\|_{L_\infty(\Omega)}^4 + 6\epsilon^{10} (\|F'(U)\|_{L_\infty(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4 + 4), \\ \tilde{\gamma}^{\text{dG}}(U) &:= 81C_P \tilde{c}^4 \|U\|_{L_\infty(\Omega)}^4, \end{aligned}$$

with $\tilde{C}_0 := (C_P^{1/2} \tilde{c}^2 + 1)/2$, $\tilde{C}_1 := (9 + 9C_P^{1/2} \tilde{c}^2 + 6^6 C_P \tilde{c}^4 + 2^{-1} 3^7 \epsilon^2)/2$ and \hat{C} the embedding constant of $\|v\|_{L_6(\Omega)} \leq \hat{C} \|\nabla v\|_{L_2(\Omega)}$.

Proof. Starting from (4.40), we shall estimate the terms I_j , $j = 6, 9, 11$ that are treated differently compared to the proof of Lemma 4.17. Using GNL ($d = 3$) we have

$$\begin{aligned} I_6^1 &\leq \frac{3}{\epsilon^2} \|\rho^3\|_{L_{4/3}(\Omega)} \|U\|_{L_\infty(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_4(\Omega)} \\ &\leq \frac{3\tilde{c}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \|U\|_{L_\infty(\Omega)} \left\| \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{1/4} \left\| \nabla \int_t^\tau \rho^2(s) ds \right\|_{L_2(\Omega)}^{3/4} \\ &\leq \frac{3\tilde{c} C_P^{1/4}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \|U\|_{L_\infty(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{4\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{3^7 C_P \tilde{c}^4}{4\epsilon^2} \|U\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4, \end{aligned}$$

and

$$\begin{aligned} I_6^2 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^2 \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \\ &\leq \frac{3C_P^{1/4} \tilde{c}}{\epsilon^2} \|\nabla \rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \|U\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \\ &\leq \frac{\epsilon^2}{2} \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{4\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{3^4 C_P \tilde{c}^4}{4\epsilon^{10}} \|U\|_{L_\infty(\Omega)}^4 \|\rho\|_{L_2(\Omega)}^4. \end{aligned}$$

Now, for I_9 we work as follows

$$\begin{aligned} I_9^1 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \|\theta\|_{L_{12}(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_6(\Omega)} \\ &\leq \frac{3\hat{C}}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^3 \|\theta\|_{L_{12}(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{4\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{3^7 \hat{C}^4}{4\epsilon^2} \|\theta\|_{L_{12}(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4, \\ I_9^2 &\leq \frac{3}{\epsilon^2} \|\rho\|_{L_4(\Omega)}^2 \|\theta\|_{L_4(\Omega)} \|\rho\|_{L_4(\Omega)} \leq \frac{1}{4\epsilon^2} \|\rho\|_{L_4(\Omega)}^4 + \frac{3^7}{4\epsilon^2} \|\theta\|_{L_4(\Omega)}^4. \end{aligned}$$

Using completely analogous arguments, we have that

$$\begin{aligned} I_{11} &\leq \epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \rho^2(s) \, ds \right\|_{L_4(\Omega)} \\ &\leq \frac{C_P^{1/4} \tilde{c}}{\epsilon^2} \|F'(U)\|_{L_\infty(\Omega)} \|\rho\|_{L_2(\Omega)} \|\rho\|_{L_4(\Omega)} \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)} \\ &\leq \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 + \frac{1}{16} \|\rho\|_{L_4(\Omega)}^4 + \frac{C_P \tilde{c}^4}{\epsilon^8} \|F'(U)\|_{L_\infty(\Omega)}^4 \left\| \int_t^\tau \nabla \rho^2(s) \, ds \right\|_{L_2(\Omega)}^4. \end{aligned}$$

Collecting all the estimates, (4.18) follows. \square

4.3.2 Spectral estimates and eigenvalue approximations

At this point, the *a posteriori* error analysis requires a lower bound for the principal eigenvalue of the linearized Allen-Cahn operator with respect to the approximate solution, $U(t)$, i.e.,

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

Thus, we seek the construction of a lower bound $-\bar{\Lambda}(t) \leq -\Lambda(t)$. Again, we assume that one of the cases of Assumption 3.11 holds, which includes the more realistic scenario that is the occurrence of topological changes.

In the vein of [BMO11, Section 3.2] and the results presented in Section 3.3.2 for linear conforming finite elements, we now investigate the hp -finite element approximation of the corresponding eigenvalue problems. Specifically, we shall compute an approximation $-\Lambda_{hp}(t)$ of $-\Lambda(t)$ using conforming hp -finite elements, and we shall obtain a lower bound $-\bar{\Lambda}(t)$ for almost all $t \in (0, T]$, upon assuming that $\|U\|_{L_\infty(\Omega)}$ remains bounded independently of $1/\epsilon$. The motivation of investigating the use of hp -version finite elements for the estimation of the required eigenvalue, is the reduction of the computational effort in line with the potentially high order version of the underlying spatial decomposition. Crucially, however, the computation of $-\Lambda_{hp}$ does *not* need to be performed on a polytopic spatial mesh, as $-\Lambda_{hp}$ is a quantity relating to the PDE problem and not of the discretization itself.

We omit the time dependence for brevity: so, for each fixed t , there exist nontrivial functions $w \in H_0^1(\Omega)$ such that, for all $v \in H_0^1(\Omega)$, we have

$$(\nabla w, \nabla v) + \epsilon^{-2} (F'(U)w, v) = -\Lambda(w, v). \quad (4.42)$$

We now investigate the approximation of the above eigenvalue problems produced by an hp -finite element method. We consider \mathcal{T}_h to be a shape-regular and conforming subdivision of domain Ω into d -simplices, τ , with $h_\tau := \text{diam}(\tau)$ and let Γ be the interior mesh skeleton of $(d-1)$ -dimensional faces, $e \subset \Gamma$. To each element $\tau \in \mathcal{T}_h$ we specify a polynomial degree $p_\tau \in \mathbb{N}$ and collect the latter in a vector $\mathbf{p} := (p_\tau : \tau \in \mathcal{T}_h)$. We define the hp -finite element space

$$S_h^{\mathbf{P}} = \{\chi \in C(\bar{\Omega}); \chi|_\tau \in \mathbb{P}_{p_\tau}(\tau), \forall \tau \in \mathcal{T}_h\},$$

with $\mathbb{P}_{p_\tau}(\tau)$ denoting the d -variate polynomials of degree at most p_τ on τ . Then, we consider the following discrete scheme of (4.42): We seek for $(w_h, \Lambda_{hp}) \in S_h^{\mathbf{P}} \times \mathbb{R}$ with $\|w_h\|_{L_2(\Omega)} = 1$ such that for all $v_h \in S_h^{\mathbf{P}}$,

$$(\nabla w_h, \nabla v_h) + \epsilon^{-2} (F'(U), v_h) = -\Lambda_{hp}(w_h, v_h). \quad (4.43)$$

Let $\Pi_p : L_2(\tau) \rightarrow \mathbb{P}_p(\tau)$ an hp -best approximation operator such that the following hp -approximation bounds hold: for $v \in H^l(\tau)$, with $l \geq 0$, and for all $\tau \in \mathcal{T}_h$, and $0 \leq q \leq l$, we have

$$\|v - \Pi_p v\|_{H^q(\tau)} \leq C_{I,5} \frac{h_\tau^{s-q}}{p_\tau^{l-q}} \|v\|_{H^l(\tau)}; \quad (4.44)$$

where $s := \min\{p_\tau + 1, l\}$ and $C_{I,5}$ is a positive constant depending only on the shape regularity of τ , see, e.g., [BS87] and [Sch98]. Furthermore, for $q = 0$ there exists a positive constant $C_{I,6}$ depending only on the shape regularity of τ

$$\|v - \Pi_p v\|_{L_2(\partial\tau)} \leq C_{I,6} \frac{h_\tau^{s-1/2}}{p_\tau^{l-1/2}} \|v\|_{H^l(\tau)}. \quad (4.45)$$

Next, we present two results analogous to [BMO11, Propositions 3.5, 3.7] about the eigenvalue error. The first result is valid under the assumption:

$$\|w_h - P_\Lambda w_h\|_{L_2(\Omega)}^2 \leq 1/2; \quad (4.46)$$

see [Lar00] for more details. Here, we denote by P_Λ , the L_2 -projection onto the the subspace of all $w \in H_0^1(\Omega)$ that satisfy (4.42).

Lemma 4.19. Let $(w_h, \Lambda_{hp}) \in S_h^{\mathbf{P}} \times \mathbb{R}$ with $\|w_h\|_{L_2(\Omega)} = 1$ satisfy (4.43). In addition, we assume that (4.46) holds. Then, upon setting

$$\begin{aligned} \eta_{\tau,l}^2 &:= \sum_{\tau \in \mathcal{T}_h} C_{I,5}^2 \frac{h_\tau^{2s}}{p_\tau^{2l}} \|-\Lambda_{hp} w_h + \Delta w_h - \epsilon^{-2} F'(U) w_h\|_{L_2(\tau)}^2 \\ &\quad + \sum_{e \in \Gamma} C_{I,6}^2 \frac{h_\tau^{2s-1}}{p_\tau^{2l-1}} \|\llbracket \nabla w_h \rrbracket\|_{L_2(e)}^2, \end{aligned}$$

with $s := \min\{p_\tau + 1, l\}$ we have the bounds

$$\Lambda - \Lambda_{hp} \leq 4\tilde{C}\eta_{\tau,1} \left((-\Lambda_{hp})_+ + \epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \right)^{1/2}, \quad \text{for } l = 1 \quad (4.47)$$

$$\Lambda - \Lambda_{hp} \leq 4\tilde{C}\eta_{\tau,2} \left(C_v + 2\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \right), \quad \text{for } l = 2, \quad (4.48)$$

where $\tilde{C} := C_\Omega$ or $C_\Omega(C_P + 1)^{1/2}$ is the constant derived when $l = 1$ is or 2, respectively, and $C_v := \inf_{v \in H_0^1(\Omega) \setminus \{0\}} \left(\|\nabla v\|_{L_2(\Omega)}^2 / \|v\|_{L_2(\Omega)}^2 \right)$.

Proof. Let $\mathcal{R}_{\Lambda_{hp}} \in H^{-1}(\Omega)$ defined through

$$\langle \mathcal{R}_{\Lambda_{hp}}, v \rangle := -\Lambda_{hp}(w_h, v) - (\nabla w_h, \nabla v) - \epsilon^{-2} (F'(U)w_h, v), \quad (4.49)$$

for all $v \in H_0^1(\Omega)$. Note that $\langle \mathcal{R}_{\Lambda_{hp}}, \chi \rangle = 0$ for all $\chi \in S_h^P$. Set $w := P_\Lambda w_h$. Then, choosing $v = w \in H_0^1(\Omega)$ in (4.49), $v = w_h \in S_h^P \subset H_0^1(\Omega)$ in (4.42) and subtracting them, gives

$$\begin{aligned} & (w, w_h)(\Lambda - \Lambda_{hp}) \\ &= \langle \mathcal{R}_{\Lambda_{hp}}, w \rangle - \langle \mathcal{R}_{\Lambda_{hp}}, \Pi_p w \rangle \\ &= -\Lambda_{hp}(w_h, w - \Pi_p w) - (\nabla w_h, \nabla(w - \Pi_p w)) - \epsilon^{-2} (F'(U)w_h, w - \Pi_p w), \end{aligned}$$

using the property $\langle \mathcal{R}_{\Lambda_{hp}}, \Pi_p w \rangle = 0$.

Continuing in standard fashion, through Hölder's inequality and applying the estimates (4.44) and (4.45), we obtain

$$\begin{aligned} (\Lambda - \Lambda_{hp})(w, w_h) &\leq \sum_{\tau \in \mathcal{T}_h} \| -\Lambda_{hp} w_h + \Delta w_h - \epsilon^{-2} F'(U) w_h \|_{L_2(\tau)} \| w - \Pi_p w \|_{L_2(\tau)} \\ &\quad + \sum_{e \in \Gamma} \| [\nabla w_h] \|_{L_2(e)} \| w - \Pi_p w \|_{L_2(e)} \\ &\leq \eta_{\tau,l} \| w \|_{H^l(\Omega)}. \end{aligned} \quad (4.50)$$

Let $l = 2$. The elliptic regularity of (4.42) implies that

$$\| w \|_{H^2(\Omega)} \leq C_\Omega \left(|-\Lambda| + \epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)} \right) \| w \|_{L_2(\Omega)}. \quad (4.51)$$

We further estimate $|-\Lambda|$ by

$$-\epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)} \leq -\Lambda \leq C_v + \epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)}. \quad (4.52)$$

Assumption (4.46) and $\| w_h \|_{L_2(\Omega)} = 1$ imply $\| w \|_{L_2(\Omega)} \leq 1$. Thus, we deduce that

$$2(w, w_h) = \| w \|_{L_2(\Omega)}^2 + \| w_h \|_{L_2(\Omega)}^2 - \| w - w_h \|_{L_2(\Omega)}^2 \geq 1/2.$$

Inserting the above bounds into (4.50) we conclude to

$$\Lambda - \Lambda_{hp} \leq 4C_\Omega \eta_{\tau,2} \left(C_v + 2\epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)} \right)^{1/2}.$$

Note that $w_h \in H_0^1(\Omega)$ and hence $-\Lambda \leq -\Lambda_{hp}$. Since $\| w \|_{L_2(\Omega)} \leq \| w_h \|_{L_2(\Omega)} = 1$ we have

$$\begin{aligned} \| \nabla w \|_{L_2(\Omega)}^2 &= -\Lambda(w, w) + \epsilon^{-2} (F'(U)w, w) \\ &\leq (-\Lambda_{hp})_+ + \epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)}. \end{aligned}$$

Thus, for $l = 1$ we obtain

$$\Lambda - \Lambda_{hp} \leq 4C_\Omega (C_P + 1)^{1/2} \eta_{\tau,1} \left((-\Lambda_{hp})_+ + 2\epsilon^{-2} \| F'(U) \|_{L_\infty(\Omega)} \right)^{1/2}.$$

□

Therefore, the assumption (4.46) is difficult to verify in practice; this is already discussed in [Bar05, Bar16].

Remark 4.20. Note that C_v , which is defined in the above lemma, coincides with the inverse of the Poincaré constant according to the given definition (2.9) associates to the class of the convex domains and is equal to $(\pi/\text{diam}(\Omega))^2$. We refer to [AD04, PW60] for detailed derivation of this sharp uniform bound.

Here, we use the abbreviations $h_{\max} := \max_{\tau \in \mathcal{T}_h} h_\tau$ and $p_{\max} := \max_{\tau \in \mathcal{T}_h} p_\tau$. We consider the *elliptic* projection, $R_h : H_0^1(\Omega) \rightarrow S_h^P$, defined by

$$(\nabla R_h v, \nabla \chi) + (R_h v, \chi) = (\nabla v, \nabla \chi) + (v, \chi), \quad \forall \chi \in S_h^P. \quad (4.53)$$

Using Aubin-Nitsche duality argument and (4.44) we deduce that for every $v \in H^l(\Omega)$

$$\|v - R_h v\|_{L_2(\Omega)} \leq C_{I,7} \frac{h_{\max}}{p_{\max}} \|v - \Pi_p v\|_{H^1(\Omega)} \leq C_{I,7} \frac{h_{\max}}{p_{\max}} \frac{h_\tau^{s-1}}{p_\tau^{l-1}} \|v\|_{H^l(\Omega)}, \quad (4.54)$$

with $C_{I,7}$ some positive constant that depends only on the domain Ω and on $C_{I,5}$.

The next lemma presents a conditional assumption between h_τ/p_τ and ϵ , that as long as it is satisfied, an estimate of the eigenvalue error is obtained.

Lemma 4.21. Let $(w_h, \Lambda_{hp}) \in S_h^P \times \mathbb{R}$ with $\|w_h\|_{L_2(\Omega)} = 1$ satisfying (4.43). Assume that $w \in H^2(\Omega)$ satisfies (4.42) and that h_τ/p_τ is such that

$$\tilde{C} C_{I,7} \left(C_v + 2\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \right) \frac{h_{\max}}{p_{\max}} \frac{h_\tau^{s-1}}{p_\tau} \leq \frac{1}{2}, \quad (4.55)$$

where $s := \min\{p_\tau + 1, 2\}$. Then, we have the estimate

$$0 \leq \Lambda - \Lambda_{hp} \leq 8\tilde{C} C_{I,7} \left(C_v + 4\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} + 1 \right)^2 \frac{h_{\max}}{p_{\max}} \frac{h_\tau^{s-1}}{p_\tau}. \quad (4.56)$$

Proof. For brevity, we set $z_\epsilon := C_v + 2\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)}$, $p_\epsilon := \epsilon^{-2} F'(U)$ and $q_\epsilon := p_\epsilon + \|p_\epsilon\|_{L_\infty(\Omega)}$. The term q_ϵ introduces a constant shift of $-\Lambda$ and $-\Lambda_{hp}$ by $\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)}$. Let $w \in H_0^1(\Omega)$ satisfy (4.42) with $\|w\|_{L_2(\Omega)} = 1$ and w_h be the minimizer of

$$v_h \mapsto (\nabla v_h, \nabla v_h) + \epsilon^{-2} (p_\epsilon v_h, v_h)$$

among all $v_h \in S_h^P$ with $\|v_h\|_{L_2(\Omega)} = 1$. Then, for all $v_h \in S_h^P$ we have

$$\begin{aligned} 0 &\leq \Lambda - \Lambda_{hp} \\ &= -\|\nabla w\|_{L_2(\Omega)}^2 - \|q_\epsilon^{1/2} w\|_{L_2(\Omega)}^2 + \|\nabla v_h\|_{L_2(\Omega)}^2 + \|q_\epsilon^{1/2} v_h\|_{L_2(\Omega)}^2 \\ &\leq 2(\nabla v_h, \nabla(v_h - w)) + 2(q_\epsilon v_h, v_h - w). \end{aligned} \quad (4.57)$$

Noting that (4.51) and (4.52) imply the inequality

$$\|w\|_{H^2(\Omega)} \leq \tilde{C} \left(C_v + 2\epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \right) = \tilde{C} z_\epsilon, \quad (4.58)$$

Additionally, from (4.52) and since $\|w\|_{L_2(\Omega)} = 1$, we have

$$\|\nabla w\|_{L_2(\Omega)}^2 \leq |\Lambda| + \epsilon^{-2} \|F'(U)\|_{L_\infty(\Omega)} \leq z_\epsilon. \quad (4.59)$$

Assumption (4.55) combined with (4.54) and (4.58) imply that,

$$\begin{aligned} & |1 - \|R_h w\|_{L_2(\Omega)}| \\ &= |\|w\|_{L_2(\Omega)} - \|R_h w\|_{L_2(\Omega)}| \leq \|w - R_h w\|_{L_2(\Omega)} \\ &\leq C_{I,7} \frac{h_{\max}}{p_{\max}} \frac{h_{\tau}^{s-1}}{p_{\tau}} \|w\|_{H^2(\Omega)} \leq \tilde{C} C_{I,7} \frac{h_{\max}}{p_{\max}} \frac{h_{\tau}^{s-1}}{p_{\tau}} z_{\epsilon} \leq \frac{1}{2}, \end{aligned} \quad (4.60)$$

and, hence, $\|R_h w\|_{L_2(\Omega)} \geq 1/2$.

Furthermore, setting $\chi = R_h w$ and $v = w$ in (4.53), applying Cauchy-Schwarz and Young's inequalities and using (4.59), yields

$$\begin{aligned} \|\nabla R_h w\|_{L_2(\Omega)}^2 + \|R_h w\|_{L_2(\Omega)}^2 &\leq \|\nabla w\|_{L_2(\Omega)}^2 + \|w\|_{L_2(\Omega)}^2 \\ &= \|\nabla w\|_{L_2(\Omega)}^2 + 1 \leq z_{\epsilon} + 1, \end{aligned}$$

Now, we choose $v_h = R_h w / \|R_h w\|_{L_2(\Omega)}$ in (4.57) and we bound each term as follows:

$$\begin{aligned} & (\nabla v_h, \nabla (v_h - w)) \\ &= \frac{1}{\|R_h w\|_{L_2(\Omega)}^2} \left((\nabla R_h w, \nabla (R_h w - w)) + (\nabla R_h w, \nabla w) \left(1 - \|R_h w\|_{L_2(\Omega)} \right) \right) \\ &= \frac{1}{\|R_h w\|_{L_2(\Omega)}^2} \left((R_h w, R_h w - w) + (\nabla R_h w, \nabla w) \left(1 - \|R_h w\|_{L_2(\Omega)} \right) \right) \\ &\leq 4 \tilde{C} C_{I,7} (z_{\epsilon} + 1) z_{\epsilon} \frac{h_{\max}}{p_{\max}} \frac{h_{\tau}^{s-1}}{p_{\tau}}. \end{aligned}$$

Working analogously, we obtain that

$$\begin{aligned} & (q_{\epsilon} v_h, v_h - w) \\ &= \frac{1}{\|R_h w\|_{L_2(\Omega)}^2} \left((q_{\epsilon} R_h w, R_h w - w) + (q_{\epsilon} R_h w, w) \left(1 - \|R_h w\|_{L_2(\Omega)} \right) \right) \\ &\leq 4 \tilde{C} C_{I,7} \|q_{\epsilon}\|_{L_{\infty}(\Omega)} z_{\epsilon} \frac{h_{\max}}{p_{\max}} \frac{h_{\tau}^{s-1}}{p_{\tau}}. \end{aligned}$$

Collecting the above bounds, we derive the eigenvalue error estimate (4.56) that is valid under the assumption (4.60). \square

4.3.3 Continuation argument

Now if any case of the Assumption 3.11, regarding the lower bound of the principal eigenvalue of the linearized Allen-Cahn operator about the approximate solution $U(t)$, holds, we obtain

$$\begin{aligned} & \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U)\rho, \rho) \\ &\geq -\bar{\Lambda}(t)(1 - \epsilon^2) \|\rho\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U)\rho, \rho). \end{aligned} \quad (4.61)$$

Inserting (4.61) into (4.17) and (4.18) for $d = 2, 3$, respectively, and applying a continuation argument as in Section 3.3.3, we are able to conclude to an analogous result to

Lemma 3.13. Indeed, let

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

$\mathcal{D}_2^{\text{dG}} := \max\{4, \alpha^{\text{dG}}(U) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 2\}$, $\mathcal{B}_2^{\text{dG}} := \max\{16\beta^{\text{dG}}(\theta, U), \gamma^{\text{dG}}(U)\}$, for $d = 2$, while for $d = 3$,

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

$\mathcal{D}_3^{\text{dG}} := \max\{4, \alpha^{\text{dG}}(U) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 3\}$, $\mathcal{B}_3^{\text{dG}} := \max\{16\tilde{\beta}^{\text{dG}}(\theta, U), \tilde{\gamma}^{\text{dG}}(U)\}$. Then, for $\bar{\mathcal{B}}_d^{\text{dG}} := \sup_{t \in [0, T]} \mathcal{B}_d^{\text{dG}}(t)$ and $E_d^{\text{dG}} = \exp\left(\int_0^T \mathcal{D}_d^{\text{dG}}(t) dt\right)$, $d = 2, 3$ we have the following estimate.

Lemma 4.22. Let $d = 2, 3$. Assume that

$$\eta_d^{\text{dG}} \leq \left(16(T+1) \bar{\mathcal{B}}_d^{\text{dG}} (E_d^{\text{dG}})^2 \right)^{-1/4} \epsilon^{d-1/2}. \quad (4.62)$$

Then, the following estimate holds

$$\begin{aligned} & \frac{1}{4(d-1)} \|\rho\|_{L_4(0,T;L_4(\Omega))}^4 + \frac{\epsilon^2}{2} \|\nabla \rho\|_{L_2(0,T;L_2(\Omega))}^2 + \sup_{t \in [0, T]} \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2 \\ & \leq 4(\eta_d^{\text{dG}})^4 E_d^{\text{dG}}. \end{aligned} \quad (4.63)$$

4.4 Fully computable upper bounds

The quantity η_d^{dG} of the estimate (4.62) of Lemma 4.22 is still not fully computable, as several norms of the quantities θ , $(\omega - \hat{U})_t$, $\mathcal{L}_1^{\text{dG}}$ and $\rho(0)$ should be further estimated. We begin by estimating the term ρ in the respective norms in an *a posteriori* fashion. To that end we obtain

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

Recalling (4.36) for $t = t_0^- = 0$ we have that

$$\theta^0 = (\hat{U}(0) - \tilde{U}(0)) + (\tilde{U}(0) - U(0)) = (\tilde{U}(0) - \tilde{U}(0)) + (\tilde{U}(0) - U(0)),$$

where we used the definition of *time reconstruction* of \tilde{U} over J_1 . Also, since $\tilde{U}(0) = u_0$ and $U(0) := P_h^0 u_0$ we conclude that $\theta^0 = u_0 - P_h^0 u_0$.

4.4.1 Time reconstruction error estimates

We present some *time reconstruction* error identities based on the representation formula of the difference $U - \hat{U}$ given in (4.24). More specifically, we have the following result.

Lemma 4.23. [GLW21, Proposition 3.4] Consider any (real) Hilbert space X , and $U|_{J_n} \in \mathbb{P}_{q_n}(J_n; X)$, $n = 1, \dots, N$ with \widehat{U} defined from U through (4.23). Then, for given $U(t_0^-) \in X$, the following approximation identities hold

$$\|\widehat{U} - U\|_{L_2(J_n; X)} = C_n^{1/2} \|[\![U]\!]_{n-1}\|_X, \quad (4.64)$$

$$\|\widehat{U} - U\|_{L_\infty(J_n; X)} = \|[\![U]\!]_{n-1}\|_X, \quad (4.65)$$

where

$$C_n := \frac{k_n(q_n + 1)}{(2q_n + 1)(2q_n + 3)}.$$

Lemma 4.24. Let $U|_{J_n} \in \mathbb{P}_{q_n}(J_n; L_p(\Omega))$, $n = 1, \dots, N$ and $2 < p < +\infty$ with \widehat{U} satisfies (4.23). Then, for given $U(t_0^-) \in L_p(\Omega)$, the following approximation inequality holds

$$\|\widehat{U} - U\|_{L_p(J_n; L_p(\Omega))} \leq C \left(\frac{q_n^{p-4}}{k_n^{p-2}} \right)^{1/2p} \|[\![U]\!]_{n-1}\|_{L_p(\Omega)}. \quad (4.66)$$

Proof. Let $2 < p < +\infty$ and for each $t \in J_n$, $n = 1, \dots, N$ we consider

$$v(t) := \int_{t_{n-1}}^t (\widehat{U} - U)^{p-1}(s) \, ds \quad \text{and we note that} \quad v_t = (\widehat{U} - U)^{p-1}(t), \quad (4.67)$$

and also we introduce the one dimensional case of the H^1 -projection,

$$\lambda_{q_n} v(t) = \int_{t_{n-1}}^t \pi_{q_n-1} v_t(s) \, ds + v(t_{n-1}^+), \quad (4.68)$$

which implies

$$\lambda_{q_n} v(t_{n-1}^+) = v(t_{n-1}^+) \quad \text{and} \quad \lambda_{q_n} v(t_n^-) = v(t_n^-), \quad (4.69)$$

see, e.g., [Sch98]. Then, we have

$$\begin{aligned} & \|\widehat{U} - U\|_{L_p(J_n; L_p(\Omega))}^p \\ &= \int_{J_n} (\widehat{U} - U, (\widehat{U} - U)^{p-1}) \, dt = \int_{J_n} (\widehat{U} - U, v_t) \, dt \\ &= \int_{J_n} (\widehat{U} - U, v_t - \pi_{q_n-1} v_t) \, dt = \int_{J_n} (\widehat{U} - U, (v - \lambda_{q_n} v)_t) \, dt \\ &= - \int_{J_n} ((\widehat{U} - U)_t, v - \lambda_{q_n} v) \, dt, \end{aligned} \quad (4.70)$$

in the last step we integrate by parts with respect to time variable and use the identities (4.69). We use the definition of the $L_2(J_n)$ -projection operator π_{q_n} and the weak representation of time reconstruction (4.23) to obtain

$$\begin{aligned} & \int_{J_n} ((\widehat{U} - U)_t, v - \lambda_{q_n} v) \, dt \\ &= \int_{J_n} ((\widehat{U} - U)_t, \pi_{q_n}(v - \lambda_{q_n} v)) \, dt \\ &= ([\![U]\!]_{n-1}, \pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+)) \\ &\leq \|[\![U]\!]_{n-1}\|_{L_p(\Omega)} \|\pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+)\|_{L_{p'}(\Omega)}, \end{aligned} \quad (4.71)$$

using Hölder's inequality with $p' = p/(p-1)$. It remains to estimate from above the term $\|\pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+)\|_{L_{p'}(\Omega)}$. To do so, we recall [GHM09, Lemma 4.1] which upon mapping the unit interval onto J_n , $n = 1, \dots, N$, gives

$$\left| \pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+) \right|^2 \leq \frac{2}{k_n} \|v - \lambda_{q_n} v\|_{L_2(J_n)} \|(v - \lambda_{q_n} v)_t\|_{L_2(J_n)}.$$

Then, we have

$$\begin{aligned} \|\pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+)\|_{L_{p'}(\Omega)}^{p'} &= \int_{\Omega} \left| \pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+) \right|^{p'} dx \\ &\leq \left(\frac{2}{k_n} \right)^{p'/2} \int_{\Omega} \left(\int_{t_{n-1}}^{t_n} (v - \lambda_{q_n} v)^2 dt \right)^{p'/4} \left(\int_{t_{n-1}}^{t_n} (v - \lambda_{q_n} v)_t^2 dt \right)^{p'/4} dx \\ &\leq C \left(\frac{2}{k_n} \right)^{p'/2} \left(\frac{k_n}{q_n} \right)^{p'/2} \int_{\Omega} \left(\int_{t_{n-1}}^{t_n} v_t^2 dt \right)^{p'/2} dx \\ &= C \left(\frac{2}{k_n} \right)^{p'/2} \left(\frac{k_n}{q_n} \right)^{p'/2} \int_{\Omega} \|v_t\|_{L_2(J_n)}^{p'} dx. \end{aligned} \quad (4.72)$$

Now we recall the inverse inequality from [BDM07, Chapter 3, (3.1)] and by the use of an affine mapping, we have

$$\|v_t\|_{L_2(J_n)} \leq C \left(\frac{2 q_n^2}{k_n} \right)^{1/p'-1/2} \|v_t\|_{L_{p'}(J_n)}. \quad (4.73)$$

Inserting the above bound into (4.72), gives

$$\|\pi_{q_n}(v - \lambda_{q_n} v)(t_{n-1}^+)\|_{L_{p'}(\Omega)} \leq C \frac{q_n^{\frac{p-4}{2p}}}{k_n^{\frac{p-2}{2p}}} \|v_t\|_{L_{p'}(J_n; L_{p'}(\Omega))}. \quad (4.74)$$

Substituting (4.74) into (4.70) and using (4.67) yields the result. \square

Lemma 4.25 (estimation of $\mathcal{L}_1^{\text{dG}}$). We have the identity

$$\|\Delta(\omega - \tilde{U})\|_{L_2(0,T; L_2(\Omega))}^2 = \sum_{n=1}^N C_n^2 \|\llbracket \widehat{U}_t + \epsilon^{-2} \pi_{q_n} F(U) - \pi_{q_n} f \rrbracket_{n-1}\|_{L_2(\Omega)}^2. \quad (4.75)$$

Proof. Note that $\Delta\omega = \Delta\widehat{\tilde{U}} = \widehat{\Delta\tilde{U}}$, since the Laplacian is time-independent. We use (4.64) for $X = L_2(\Omega)$ to obtain

$$\begin{aligned} &\int_0^T \|\widehat{\Delta\tilde{U}} - \Delta\tilde{U}\|_{L_2(\Omega)}^2 dt \\ &= \sum_{n=1}^N \|\widehat{\Delta\tilde{U}} - \Delta\tilde{U}\|_{L_2(J_n; L_2(\Omega))}^2 = \sum_{n=1}^N C_n^2 \|\llbracket \Delta\tilde{U} \rrbracket_{n-1}\|_{L_2(\Omega)}^2 \\ &= \sum_{n=1}^N C_n^2 \|\llbracket \widehat{U}_t + \epsilon^{-2} \pi_{q_n} F(U) - \pi_{q_n} f \rrbracket_{n-1}\|_{L_2(\Omega)}^2; \end{aligned}$$

whereby in the last step we used the pointwise form (4.34) for each $n = 1, \dots, N$. \square

4.4.2 Spatial error estimates

We now estimate Θ_1^{dG} and Θ_2^{dG} (or $\tilde{\Theta}_2^{\text{dG}}$), which represent the spatial error due to the presence of the several norms of the terms θ and $(\omega - \widehat{U})_t$. We begin by justifying the characterization *spatial error* for $(\omega - \widehat{U})_t$: in view of (4.23) we have directly on J_n ,

$$\begin{aligned} (\omega - \widehat{U})_t &= (\widehat{\widetilde{U}} - U)_t = (\widetilde{U} - U)_t + \chi_n (\llbracket \widetilde{U} - U \rrbracket_{n-1}) \\ &= (\widetilde{U} - U)_t + \varkappa_n(t) \llbracket \widetilde{U} - U \rrbracket_{n-1}. \end{aligned} \quad (4.76)$$

Then, it follows that

$$\|(\omega - \widehat{U})_t\|_{L_p(\Omega)} \leq \|\widetilde{U}_t - U_t\|_{L_p(\Omega)} + |\varkappa_n(t)| \|\llbracket \widetilde{U} - U \rrbracket_{n-1}\|_{L_p(\Omega)}, \quad t \in J_n, \quad (4.77)$$

where $\llbracket \widetilde{U} - U \rrbracket_{n-1} = (\widetilde{U} - U)(t_{n-1}^+) - (\widetilde{U} - U)(t_{n-1}^-)$.

From (4.30), for each $t \in J_n$, $U \in S_h^n$ is the spatial dG-approximation of \widetilde{U} . Differentiating (4.26) with respect to the time variable and since the elliptic operator is t -independent, U_t is the spatial dG-approximation of \widetilde{U}_t . Assuming the availability of estimators of the form (4.31) for both *elliptic reconstruction errors*, $\widetilde{U} - U$ and $\widetilde{U}_t - U_t$, we have

$$\begin{aligned} \|(\omega - \widehat{U})_t\|_{L_p(\Omega)} &\leq \mathcal{E}(U_t, g_t^n(t); L_p(\Omega)) + |\varkappa_n(t)| \mathcal{E}(U_{n-1}^-, g^{n-1}(t_{n-1}^-); L_p(\Omega)) \\ &\quad + |\varkappa_n(t)| \mathcal{E}(U_{n-1}^+, g^n(t_{n-1}^+); L_p(\Omega)), \end{aligned}$$

where $U_{n-1}^- \in S_h^{n-1}$ and $U_{n-1}^+ \in S_h^n$.

To estimate θ , we recall (4.36) and use the triangle inequality to obtain

$$\int_0^T \|\theta\|_{L_p(\Omega)}^p dt \leq 2^{p-1} \left(\int_0^T \|\widehat{\widetilde{U}} - \widetilde{U}\|_{L_p(\Omega)}^p dt + \int_0^T \|\widetilde{U} - U\|_{L_p(\Omega)}^p dt \right). \quad (4.78)$$

The computable upper bounds over each J_n , presented in Lemma 4.23, give

$$\begin{aligned} \int_0^T \|\widehat{\widetilde{U}} - \widetilde{U}\|_{L_p(\Omega)}^p dt &= \sum_{n=1}^N \|\widehat{\widetilde{U}} - \widetilde{U}\|_{L_p(J_n; L_p(\Omega))}^p \leq \sum_{n=1}^N C_n^p \|\llbracket \widetilde{U} \rrbracket_{n-1}\|_{L_p(\Omega)}^p \\ &\leq 2^{p-1} \sum_{n=1}^N C_n^p \left(\|\llbracket U \rrbracket_{n-1}\|_{L_p(\Omega)}^p + \|\llbracket \widetilde{U} - U \rrbracket_{n-1}\|_{L_p(\Omega)}^p \right). \end{aligned}$$

Inserting the above result into (4.78) and assuming that (4.31) holds, we deduce

$$\begin{aligned} &\|\theta\|_{L_p(0, T; L_p(\Omega))}^p \\ &\leq 2^{2p-2} \sum_{n=1}^N C_n^p \left[\mathcal{E}^p(U_{n-1}^+, g^n(t_{n-1}^+); L_p(\Omega)) + \mathcal{E}^p(U_{n-1}^-, g^{n-1}(t_{n-1}^-); L_p(\Omega)) \right. \\ &\quad \left. + \|\llbracket U \rrbracket_{n-1}\|_{L_p(\Omega)}^p \right] + 2^{p-1} \sum_{n=1}^N \int_{J_n} \mathcal{E}^p(U(t), g^n(t); L_p(\Omega)) dt, \end{aligned}$$

for $p \in [2, +\infty)$.

4.4.3 Elliptic reconstruction error estimates

Next, we focus on the derivation of *a posteriori* error estimators of the form

$$\|\tilde{U}(t) - U(t)\|_{L_p(\Omega)} \leq \mathcal{E}(U(t), g^n(t); L_p(\Omega)),$$

for all $t \in J_n, n = 1, \dots, N$ and $p \geq 2$, whose availability is postulated in the previous section. To that end, we consider the dual problem:

$$-\Delta z = \psi^{p-1} \quad \text{in } \Omega, \quad z = 0 \quad \text{on } \partial\Omega. \quad (4.79)$$

Elliptic regularity asserts that there exists a constant $C_\Omega > 0$, depending only on the domain Ω , such that

$$\|z\|_{W^{2,p/(p-1)}(\Omega)} \leq C_\Omega \|\psi^{p-1}\|_{L_{p/(p-1)}(\Omega)} = C_\Omega \|\psi\|_{L_p(\Omega)}^{p-1}, \quad \text{for } p \geq 2, \quad (4.80)$$

we refer to [Gri11] for details. Combining (4.4) with the approximation results (4.7) and (4.8) for $q = p/(p-1)$, we deduce that for all $z \in W^{2,p/(p-1)}(\tau)$ there holds

$$\|z - \Pi_1 z\|_{L_{p/(p-1)}(\partial\tau)} \leq \mathcal{C}_1 h_\tau^{(p+1)/p} |z|_{W^{2,p/(p-1)}(\tau)}, \quad (4.81)$$

$$\|\nabla(z - \Pi_1 z)\|_{L_{p/(p-1)}(\partial\tau)} \leq \mathcal{C}_2 h_\tau^{1/p} |z|_{W^{2,p/(p-1)}(\tau)}, \quad (4.82)$$

here $\mathcal{C}_1, \mathcal{C}_2$ positive constants depending on C_{tr} and $C_{\hat{P}}$ only.

Set $\psi = \tilde{U}(t) - U(t), t \in J_n, n = 1, \dots, N$ in the dual problem (4.79). Applying the Divergence Theorem on every elemental integral, since U is elementwise continuous, we have that

$$\begin{aligned} \|\tilde{U} - U\|_{L_p(\Omega)}^p &= \int_{\Omega} |\tilde{U} - U| |\tilde{U} - U|^{p-1} dx = - \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \Delta z |\tilde{U} - U| dx \\ &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla(U - \tilde{U}) \cdot \nabla z dx - \sum_{\tau \in \mathcal{T}_h^n} \int_{\partial\tau} (\nabla z \cdot \mathbf{n})(U - \tilde{U}) ds. \end{aligned}$$

Setting $V_h = \Pi_1 z$ in (4.32) and subtracting it from the last relation, we obtain after some standard manipulations

$$\begin{aligned} &\|\tilde{U} - U\|_{L_p(\Omega)}^p \\ &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla(\tilde{U} - U) \cdot \nabla(z - \Pi_1 z) dx + \int_{\Gamma^n} [\![U]\!] \cdot \{\nabla(z - \Pi_1 z)\} ds \\ &\quad - \int_{\Gamma^n} \sigma [\![U]\!] \cdot [\![z - \Pi_1 z]\!] ds + \int_{\Gamma^n} \{\nabla(\tilde{U} - U)\} \cdot [\![z - \Pi_1 z]\!] ds. \end{aligned} \quad (4.83)$$

Applying elementwise integration by parts on the first term on the right-hand side of (4.83) and recalling (4.29), we arrive to

$$\begin{aligned} &\sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla(\tilde{U} - U) \cdot \nabla(z - \Pi_1 z) dx \\ &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} (g^n + \Delta U)(z - \Pi_1 z) dx + \int_{\Gamma^n} \{\nabla \tilde{U}\} \cdot [\![z - \Pi_1 z]\!] ds \\ &\quad - \sum_{\tau \in \mathcal{T}_h^n} \int_{\partial\tau} (\nabla U \cdot \mathbf{n})(z - \Pi_1 z) ds. \end{aligned}$$

Using the well-known elementary identity

$$\begin{aligned} & \sum_{\tau \in \mathcal{T}_h^n} \int_{\partial\tau} (\nabla U \cdot \mathbf{n})(z - \Pi_1 z) \, ds \\ &= \int_{\Gamma^n} \{\nabla U\} \cdot [\![z - \Pi_1 z]\!] \, ds + \int_{\Gamma_{int}^n} [\![\nabla U]\!] \cdot \{z - \Pi_1 z\} \, ds, \end{aligned}$$

and combining the above we arrive at

$$\begin{aligned} \|\tilde{U} - U\|_{L_p(\Omega)}^p &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} (g^n + \Delta U)(z - \Pi_1 z) \, dx - \int_{\Gamma_{int}^n} [\![\nabla U]\!] \cdot \{z - \Pi_1 z\} \, ds \\ &\quad + \int_{\Gamma^n} [\![U]\!] \cdot \{\nabla(z - \Pi_1 z)\} \, ds - \int_{\Gamma^n} \sigma [\![U]\!] \cdot [\![z - \Pi_1 z]\!] \, ds \\ &:= \sum_{i=1}^4 \Phi_i. \end{aligned}$$

We shall further estimate each Φ_i separately. In the following approximation results we recall the mesh-function h such that $h|_{\tau} = h_{\tau}$ while $h|_e = \max_{e=\partial\tau \cap \partial\tau'} \{h_{\tau}, h_{\tau'}\}$ for $\tau, \tau' \in \mathcal{T}_h^n$. Beginning with Φ_1 , we apply Hölder's inequality and from (4.7) with $q = p/(p-1)$, respectively,

$$\begin{aligned} \Phi_1 &\leq \sum_{\tau \in \mathcal{T}_h^n} \|g^n + \Delta U\|_{L_p(\tau)} \|z - \Pi_1 z\|_{L_{\frac{p}{p-1}}(\tau)} \\ &\leq \sum_{\tau \in \mathcal{T}_h^n} \|g^n + \Delta U\|_{L_p(\tau)} C_P^2 h^2 \|z\|_{W^{2, \frac{p}{p-1}}(\tau)} \\ &\leq \left(\sum_{\tau \in \mathcal{T}_h^n} C_{I_1} \|h^2(g^n + \Delta U)\|_{L_p(\tau)}^p \right)^{\frac{1}{p}} \|z\|_{W^{2, \frac{p}{p-1}}(\Omega)}. \end{aligned}$$

Hölder's inequality and the trace estimate (4.81) also yield

$$\begin{aligned} \Phi_2 &\leq \sum_{e \in \Gamma_{int}^n} \|[\![\nabla U]\!]\|_{L_p(e)} \|\{z - \Pi_1 z\}\|_{L_{\frac{p}{p-1}}(e)} \\ &\leq \left(\sum_{e \in \Gamma_{int}^n} h^{p+1} \|[\![\nabla U]\!]\|_{L_p(e)}^p \right)^{\frac{1}{p}} \left(\sum_{\tau \in \mathcal{T}_h^n} h^{-\frac{p+1}{p-1}} \|z - \Pi_1 z\|_{L_{\frac{p}{p-1}}(\partial\tau)}^{\frac{p}{p-1}} \right)^{\frac{p-1}{p}} \\ &\leq \left(\sum_{e \in \Gamma_{int}^n} C_{I_2} \|h^{1+\frac{1}{p}} [\![\nabla U]\!]\|_{L_p(e)}^p \right)^{\frac{1}{p}} \|z\|_{W^{2, \frac{p}{p-1}}(\Omega)}. \end{aligned}$$

In the same spirit, we have

$$\begin{aligned} \Phi_3 &\leq \sum_{e \in \Gamma} \|[\![U]\!]\|_{L_p(e)} \|\{\nabla(z - \Pi_1 z)\}\|_{L_{\frac{p}{p-1}}(e)} \\ &\leq \left(\sum_{e \in \Gamma} h \|[\![U]\!]\|_{L_p(e)}^p \right)^{\frac{1}{p}} \left(\sum_{\tau \in \mathcal{T}_h^n} h^{-\frac{1}{p-1}} \|\nabla(z - \Pi_1 z)\|_{L_{\frac{p}{p-1}}(\partial\tau)}^{\frac{p}{p-1}} \right)^{\frac{p-1}{p}} \\ &\leq \left(\sum_{e \in \Gamma} C_{I_3} \|h^{\frac{1}{p}} [\![U]\!]\|_{L_p(e)}^p \right)^{\frac{1}{p}} \|z\|_{W^{2, \frac{p}{p-1}}(\Omega)}, \end{aligned}$$

applying trace estimate (4.82). Finally, we bound the last term as follows:

$$\begin{aligned}\Phi_4 &\leq \sum_{e \in \Gamma} \sigma \|[\![U]\!]_{L_p(e)} \| [\![z - \Pi_1 z]\!]_{L^{\frac{p}{p-1}}(e)} \\ &\leq \left(\sum_{e \in \Gamma} \sigma^p h^{p+1} \|[\![U]\!]_{L_p(e)}^p \right)^{\frac{1}{p}} \left(\sum_{\tau \in \mathcal{T}_h^n} h^{-\frac{p+1}{p-1}} \|z - \Pi_1 z\|_{L^{\frac{p}{p-1}}(\partial\tau)}^{\frac{p}{p-1}} \right)^{\frac{p-1}{p}} \\ &\leq \left(\sum_{e \in \Gamma} C_{I_4} \sigma^p \|h^{1+\frac{1}{p}} [\![U]\!]_{L_p(e)}^p \right)^{\frac{1}{p}} \|z\|_{W^{2,\frac{p}{p-1}}(\Omega)}.\end{aligned}$$

Collecting all these bounds and using elliptic regularity (4.80), we conclude to the following *a posteriori* error estimator

$$\begin{aligned}&\|\tilde{U} - U\|_{L_p(\Omega)} \\ &\leq C_\Omega \left(\sum_{\tau \in \mathcal{T}_h^n} C_{I_1} \|h_\tau^2 (g^n + \Delta U)\|_{L_p(\tau)}^p + \sum_{e \in \Gamma_{int}^n} C_{I_2} \|h_\tau^{1+\frac{1}{p}} [\!\nabla U]\!]_{L_p(e)}^p \right. \\ &\quad \left. + \sum_{e \in \Gamma^n} C_{I_3} \|h_\tau^{\frac{1}{p}} [\![U]\!]_{L_p(e)}^p + \sum_{e \in \Gamma^n} C_{I_4} \sigma^p \|h_\tau^{1+\frac{1}{p}} [\![U]\!]_{L_p(e)}^p \right)^{\frac{1}{p}} \\ &:= \mathcal{E}(U(t), g^n(t); L_p(\Omega)),\end{aligned}\tag{4.84}$$

for all $t \in J_n$, $n = 1, \dots, N$.

4.5 Main Results

Now we shall present an analogous *a posteriori* error estimate in the $L_4(0, T; L_4(\Omega))$ -norm to Theorem 3.14 of Chapter 3. The enhanced regularity of the data, i.e., forcing term f and initial condition u_0 , that is presented below, guarantees the desired regularity of the solution: $u \in L_4(0, T; W^{2,4}(\Omega))$ and $u_t \in L_4(0, T; L_4(\Omega))$. As we already discussed in Remark 3.15, we have to enforce the aforementioned regularity in order to validate the choice of the test function.

Theorem 4.26. Let $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ and $f \in L_\infty(0, T; L_4(\Omega))$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. Let also u be the solution of (3.1) and U is its approximate solution (4.11). Assume that (3.11)(II) and the conditions (4.62) are satisfied. Then, there holds

$$\|u - U\|_{L_4(0, T; L_4(\Omega))} \leq 2\eta_d^{\text{dG}} ((d-1)E_d^{\text{dG}})^{1/4} + \|\theta\|_{L_4(0, T; L_4(\Omega))}.\tag{4.85}$$

Proof. Ignoring nonnegative terms on the left-hand side of (4.63), we have

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

Then, recalling the error decomposition (4.35) and applying the triangle inequality the estimate (4.85) is derived directly. \square

Remark 4.27. The above estimate holds under the most realistic scenario, Assumption 3.11(II), where topological changes take place. Although, we note that the Theorem 4.26 is still valid when the evolving interfaces are smooth and Assumption 3.11(I) holds. Particularly, we replace $E_d^{\text{dG}} = \exp\left(\int_0^T \mathcal{D}_d^{\text{dG}}(t) dt\right)$ by $E_d^{\text{dG}} = \exp(\bar{\mathcal{D}}_d^{\text{dG}} T)$, with $\bar{\mathcal{D}}_d^{\text{dG}} := \sup_{t \in [0, T]} \max\{4, \alpha^{\text{dG}}(U) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + d\}$, $d = 2, 3$.

In the vein of [Che94, MS95] when the developed interfaces are smooth, we may expect that $E_d^{\text{DG}} \sim 1$. In the case of topological changes, based on [BMO11], we have that $E_d^{\text{DG}} \sim \epsilon^{-m}$, $m > 0$. In particular, E_d^{DG} does not grow exponentially in $1/\epsilon$. Upon setting for our convenience $C_d^{\text{dG}} := (16(T+1)\bar{B}_d^{\text{dG}})^{-1/4}$, condition (4.62) can be written as it follows:

$$\eta_d^{\text{dG}} \leq C_d^{\text{dG}} \epsilon^{d+(m-1)/2}, \quad \text{for } d = 2, 3, \text{ and, } m \geq 0$$

considering both cases of Assumption 3.11 about the availability and the properties of a lower bound, $-\bar{\Lambda}$, of the principal eigenvalue which underpin of the nature of the evolving interfaces.

Seeking to prove *a posteriori* error estimate in $L_4(0, T; L_4(\Omega))$ -norm, we also derived *a posteriori* error bounds in $L_2(0, T; H^1(S))$ - and $L_\infty(0, T; L_2(\Omega))$ -norms, where $S =: S_h + H_0^1(\Omega)$ endowed with the corresponding dG-norm.

Proposition 4.28. Under the hypotheses of Theorem 4.26 and, upon assuming condition (4.62) that implies

$$\hat{\eta}_d^{\text{dG}} := (\eta_d^{\text{dG}})^2 \leq (G_d^{\text{dG}})^2 \epsilon^{2d-1+m},$$

the following error bounds hold

$$\begin{aligned} \|u - U\|_{L_\infty(0, T; L_2(\Omega))} &\leq 2\sqrt{2E_d^{\text{dG}}} \hat{\eta}_d^{\text{dG}} + \|\theta\|_{L_\infty(0, T; L_2(\Omega))}, \\ \|u - U\|_{L_2(0, T; H^1(S))} &\leq \epsilon^{-1} 2\sqrt{2E_d^{\text{dG}}} \hat{\eta}_d^{\text{dG}} + \|\theta\|_{L_2(0, T; H^1(S))}. \end{aligned}$$

Thus we managed to extend the *a posteriori* bounds applied in Chapter 3 for the simpler fully discrete scheme to the case of the space-time discontinuous method of arbitrary order. The decomposition of the spatial domain into general polytopes demands a lot of carefully constructed technical tools in order to derive approximation results under the ‘new’ mesh regularity properties. To the best of our knowledge, the above *a posteriori* error bounds in $L_4(0, T; L_4(\Omega))$ -, $L_\infty(0, T; L_2(\Omega))$ -, and $L_2(0, T; H^1(S))$ -norms are the first results of *a posteriori* error analysis discontinuous Galerkin methods for the Allen-Cahn problem and are inclusive at the incorporation of polytopic meshes. The conditional type estimators depend polynomially on the inverse of the interface length, $1/\epsilon$. Crucially, the estimator η_d^{dG} satisfies the condition (4.62), which exhibits an analogously favourable ϵ -dependence to the corresponding condition in Chapter 3. The latter justifies our interest to investigate $L_4(0, T; L_4(\Omega))$ -norm *a posteriori* error bounds for the Allen-Cahn problem. Thus, we conclude that the non-standard energy argument of Chapter 3 is generic enough to allow for the proof of *a posteriori* error estimators simultaneously in $L_4(0, T; L_4(\Omega))$ -, $L_\infty(0, T; L_2(\Omega))$ - and $L_2(0, T; H^1(S))$ -norms for arbitrary order space-time dG methods under less stringent conditions compared to the results of [BMO11, BM11] for low order schemes.

CHAPTER 5

OPTIMAL CONTROL PROBLEM

This chapter is devoted to the minimization of

$$\begin{aligned} J(u) = & \frac{1}{2} \int_0^T \int_{\Omega} |y_u(t, x) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_{\Omega} |y_u(T, x) - y_{\Omega}(x)|^2 dx \\ & + \frac{\mu}{2} \int_0^T \int_{\Omega} |u(t, x)|^2 dx dt, \end{aligned} \quad (5.1)$$

subject to

$$\begin{aligned} y_{u,t} - \Delta y_u + \frac{1}{\epsilon^2} (y_u^3 - y_u) &= u && \text{in } \Omega_T = \Omega \times (0, T), \\ y_u &= 0 && \text{on } \Sigma_T = \partial\Omega \times (0, T), \\ y_u(\cdot, 0) &= y_0 && \text{in } \Omega. \end{aligned} \quad (5.2)$$

We present a detailed analysis of the optimal control problem formulated, in the standard reduced functional form, as

$$\left\{ \begin{array}{l} \min J(u) \\ u \in U_{ad}, \end{array} \right. \quad (5.3)$$

where

$$U_{ad} = \left\{ u \in L_2(0, T; L_2(\Omega)) ; u_a \leq u(t, x) \leq u_b \text{ for a.e. } (t, x) \in \Omega_T \right\},$$

is the set of admissible controls. Specifically, we shall study both the control to state, and of the state to adjoint mappings and shall derive first and second order optimality conditions that is crucial due to the non-convexity of the optimal control problem. In particular, under a closeness assumption on the controls, we establish the Lipschitz continuity of the control to state mapping, with Lipschitz constant that is independent of ϵ in the $L_{\infty}(0, T; L_2(\Omega))$ and $L_2(0, T; H_0^1(\Omega))$ norms by exploiting the presence of $L_4(0, T; L_4(\Omega))$ critical term, the *spectral estimate* at a ‘continuous level’ and the *nonlinear Gronwall Lemma*. For the state to adjoint mapping, using similar technical tools we are able to obtain Lipschitz results with constants that depend *polynomially* upon $1/\epsilon$.

5.1 Preliminary setting

Let $\Omega \subset \mathbb{R}^d$ be a convex, polygonal ($d = 2$) or polyhedral ($d = 3$) domain of the Euclidean space \mathbb{R}^d and $T \in \mathbb{R}^+$ the final time. We will use the notation of Chapters 3 and 4 regarding the Sobolev and Bochner spaces and their corresponding norms. We also consider the functional space

$$W_p^{2,1}(\Omega_T) = \left\{ v \in L_p(\Omega_T) : \frac{\partial v}{\partial x_i}, \frac{\partial^2 v}{\partial x_i \partial x_j}, \frac{\partial v}{\partial t} \in L_p(\Omega_T), 1 \leq i, j \leq d \right\},$$

with the respective norm

$$\begin{aligned} \|v\|_{W_p^{2,1}(\Omega_T)} &= \left\{ \int_{\Omega_T} \left(|v|^p + \left| \frac{\partial v}{\partial t} \right|^p \right) dx dt \right. \\ &\quad \left. + \sum_{i=1}^d \int_{\Omega_T} \left| \frac{\partial v}{\partial x_i} \right|^p dx dt + \sum_{i,j=1}^d \int_{\Omega_T} \left| \frac{\partial^2 v}{\partial x_i \partial x_j} \right|^p dx dt \right\}^{1/p}. \end{aligned}$$

We adopt the notation: $H^{2,1}(\Omega_T) := W_2^{2,1}(\Omega_T)$. Furthermore, we consider the set $W(0, T) := \left\{ v \in L_2(0, T; H_0^1(\Omega)), v_t \in L_2(0, T; H^{-1}(\Omega)) \right\}$. We will use extensively the classical *interpolation inequality* for all $v \in L_4(\Omega)$,

$$\|v\|_{L_3(\Omega)}^3 \leq \|v\|_{L_2(\Omega)} \|v\|_{L_4(\Omega)}^2, \quad \text{for } d = 2, 3, \quad (5.4)$$

Throughout the remaining of Chapters 5 and 6 we adopt the standard notation for the control and $y := y_u$ for its associated state. Assume that $u \in L_2(0, T; L_2(\Omega))$, $y_0 \in L_2(\Omega)$, $y_\Omega \in H_0^1(\Omega)$. The weak formulation of the state equation (5.2) becomes: We seek $y \in W(0, T)$ such that for a.e. $t \in (0, T)$,

$$\begin{aligned} \langle y_t, v \rangle + (\nabla y, \nabla v) + \epsilon^{-2} (y^3 - y, v) &= (u, v), \\ (y(0), v) &= (y_0, v), \end{aligned} \quad (5.5)$$

for all $v \in H_0^1(\Omega)$. Recall that for any $\epsilon > 0$, and $y_0 \in H_0^1(\Omega)$, it is easy to show that $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ (see [Tem97]). We refer the readers to [Tem97, Zei90] for straightforward techniques that prove the enhanced regularity results. The following lemma quantifies the dependence upon ϵ of various norms.

Lemma 5.1. 1. Let $u \in L_2(0, T; L_2(\Omega))$ and $y_0 \in L_2(\Omega)$. Then, there exists a constant $C > 0$ independent of ϵ , such that:

$$\begin{aligned} &\|y\|_{L_2(0, T; L_2(\Omega))} + \|y\|_{L_4(0, T; L_4(\Omega))}^2 \\ &\leq C \left(|\Omega_T|^{\frac{1}{2}} + \epsilon \|y_0\|_{L_2(\Omega)} + \epsilon^2 \|u\|_{L_2(0, T; L_2(\Omega))} \right) =: C_{st,1}, \\ &\|y\|_{L_\infty(0, T; L_2(\Omega))} + \|y\|_{L_2(0, T; H^1(\Omega))} \leq \frac{C_{st,1}}{\epsilon}. \end{aligned}$$

2. Let $u \in L_2(0, T; L_2(\Omega))$ and $y_0 \in H_0^1(\Omega)$. Then, there exists a constant $C > 0$

independent of ϵ , such that the following estimates hold:

$$\begin{aligned} & \|y\|_{L_\infty(0,T;H^1(\Omega))} + \|y_t\|_{L_2(0,T;L_2(\Omega))} + \frac{1}{2\epsilon} \|(y^2 - 1)^2\|_{L_\infty(0,T;L_1(\Omega))}^{1/2} \\ & \leq C \left(\|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{st,2}, \\ & \|y\|_{L_2(0,T;H^2(\Omega))} \leq C \left(\frac{T^{1/2}C_{st,2}}{\epsilon} + \|\nabla y_0\|_{L_2(\Omega)} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{st,3}. \end{aligned}$$

Proof. These estimates are standard (see e.g. [FP03, Bar16, Chr19]). For completeness we state the main steps of their proofs. For the first result, testing (5.5) against y , and using Young's inequalities, we obtain

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|y\|_{L_2(\Omega)}^2 + \|\nabla y\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} \|y\|_{L_4(\Omega)}^4 \leq \frac{2}{\epsilon^2} \|y\|_{L_2(\Omega)}^2 + \frac{\epsilon^2}{4} \|u\|_{L_2(\Omega)}^2 \\ & \leq \frac{1}{2\epsilon^2} \|y\|_{L_4(\Omega)}^4 + \frac{2}{\epsilon^2} |\Omega| + \frac{\epsilon^2}{4} \|u\|_{L_2(\Omega)}^2. \end{aligned}$$

Integrating from 0 to T and standard algebra we get the estimate in $L_4(0, T; L_4(\Omega))$ -norm. Integrating from 0 to t , and using the bound of $\|y\|_{L_4(0,T;L_4(\Omega))}$, we deduce the estimate in $L_\infty(0, T; L_2(\Omega))$ -norm. Note that Hölder and Young's inequalities yield

$$\begin{aligned} \|y\|_{L_2(0,T;L_2(\Omega))} & \leq |\Omega|^{1/4} T^{1/4} \|y\|_{L_4(0,T;L_4(\Omega))} \\ & \leq C \left(|\Omega|^{1/2} T^{1/2} + \|y\|_{L_4(0,T;L_4(\Omega))}^2 \right). \end{aligned}$$

Now we test (5.5) against y_t , and we use Young's inequality to get

$$\|y_t\|_{L_2(\Omega)}^2 + \frac{d}{dt} \left(\frac{1}{2} \|\nabla y\|_{L_2(\Omega)}^2 + \frac{1}{4\epsilon^2} \|(y^2 - 1)^2\|_{L_1(\Omega)} \right) \leq \frac{1}{2} \|y_t\|_{L_2(\Omega)}^2 + \frac{1}{2} \|u\|_{L_2(\Omega)}^2.$$

Integrating with respect to $t \in (0, \tau)$, we obtain

$$\begin{aligned} & \|y_t\|_{L_2(0,\tau;L_2(\Omega))}^2 + \|\nabla y(\tau)\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \|(y^2(\tau) - 1)^2\|_{L_1(\Omega)} \\ & \leq \|u\|_{L_2(0,\tau;L_2(\Omega))}^2 + \|\nabla y(0)\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \|(y^2(0) - 1)^2\|_{L_1(\Omega)}, \end{aligned} \tag{5.6}$$

which implies the desired estimate. Testing (5.2) against $-\Delta y$, integrating by parts with respect to space, and Young's inequality yield

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|\nabla y\|_{L_2(\Omega)}^2 + \|\Delta y\|_{L_2(\Omega)}^2 + \frac{3}{\epsilon^2} \|y \nabla y\|_{L_2(\Omega)}^2 \\ & \leq \frac{1}{2} \left(\|\Delta y\|_{L_2(\Omega)}^2 + \|u\|_{L_2(\Omega)}^2 \right) + \frac{1}{\epsilon^2} \|\nabla y\|_{L_2(\Omega)}^2. \end{aligned}$$

The estimate is completed after integrating with respect to time and substituting the bounds of $\|\nabla y\|_{L_\infty(0,T;L_2(\Omega))}$.

Remark 5.2. At this point, it is of crucial importance for the upcoming analysis to deduce that $y \in L_\infty(0, T; L_\infty(\Omega))$. Indeed, we obtain that since the controls satisfy point-wise constraints, i.e., the set of admissible controls is defined as a subset of $L_\infty(0, T; L_\infty(\Omega))$. We assume that $y_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$, where $W^{1,4}(\Omega) \subset L_\infty(\Omega)$. Then, according to maximal parabolic regularity we may deduce that $y \in L_\infty(0, T; L_\infty(\Omega))$.

□

Remark 5.3. Note that, if

$$\|\nabla y(0)\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y^2(0) - 1)^2\|_{L_1(\Omega)}^{1/2} \leq D,$$

holds with D independent of ϵ , then the constant $C_{st,2}$ of Lemma 5.1 is bounded independently of ϵ and, hence, we deduce

$$\|y\|_{H^{2,1}(\Omega_T)} \leq \frac{C}{\epsilon} (D + \|u\|_{L_2(0,T;L_2(\Omega))}),$$

where C is an algebraic constant depending only on the domain Ω . The condition

$$\|\nabla y(0)\|_{L_2(\Omega)}^2 + \frac{1}{4\epsilon^2} \|(y^2(0) - 1)^2\|_{L_1(\Omega)} \leq D^2$$

relates to the assumption that the associated Ginzburg-Landau energy is bounded at 0. This assumption is commonly used in the literature, see for instance [FP03], and it takes the form of:

$$\|\nabla y(0)\|_{L_2(\Omega)}^2 + \frac{1}{4\epsilon^2} \|(y^2(0) - 1)^2\|_{L_1(\Omega)} \leq C\epsilon^{-\sigma_1}, \quad \text{for some } \sigma_1 \geq 0.$$

Indeed, for the uncontrolled problem with zero Neumann boundary data and initial data $y_0 \in H_0^1(\Omega)$, the solution of (5.2) satisfies, for any $t \geq 0$,

$$\frac{d}{dt} E(t) + \|y_t(t)\|_{L_2(\Omega)}^2 = 0 \tag{5.7}$$

where $E(t)$ denotes the associated Ginzburg-Landau energy that is, for a.e. $t \in (0, T]$,

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

As a consequence, (5.7), implies that $E(s) \leq E(0)$, for every $s \in (0, T]$.

5.2 Optimality conditions

This section is devoted to the analysis of optimal control (5.3). Since we are dealing with a non-convex optimal control problem, the first order necessary optimality conditions are no longer sufficient. Consequently, we need to consider sufficient second order optimality conditions for the local optimal solution.

5.2.1 Continuity

We begin by studying the continuity of the relation between the control and the state. The emphasis here is on quantifying the dependence of various Lipschitz constants upon ϵ .

Definition 5.4. The mapping $G : L_2(0, T; L_2(\Omega)) \rightarrow H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ that assigns each control function u to the corresponding state $y_u = y(u) = G(u)$, is called control to state operator.

Throughout the analysis we use the abbreviation: $F(y) := y^3 - y$ and for $u_i \in L_2(0, T; L_2(\Omega))$, $i = 1, 2$, we denote by $y_i = G(u_i) := y_{u_i}$.

Theorem 5.5. Assume that

$$\begin{aligned} \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))} &\leq \frac{\epsilon^3 \|y\|_{L_\infty(0, T; L_\infty(\Omega))}^{-1}}{12\tilde{c}(T+1)} E^{-1}, \quad \text{for } d=2, \\ \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))} &\leq \frac{\epsilon^4 \|y\|_{L_\infty(0, T; L_\infty(\Omega))}^{-1}}{48\tilde{c}(T+1)} E^{-3/2}, \quad \text{for } d=3, \end{aligned} \quad (5.8)$$

where $E := \exp(\int_0^T 2\lambda(t)(1-\epsilon^2) + (6-d) dt)$. Then, for $L_1 := 2E^{1/2}$, we have

$$\begin{aligned} &\sup_{t \in [0, T]} \|y_1 - y_2\|_{L_2(\Omega)} + \epsilon \|y_1 - y_2\|_{L_2(0, T; H_0^1(\Omega))} + \epsilon^{-1} \|y_1 - y_2\|_{L_4(0, T; L_4(\Omega))}^2 \\ &\leq L_1 \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))}. \end{aligned} \quad (5.9)$$

Proof. Subtracting the equations satisfied by y_1 and y_2 , it yields that

$$\begin{aligned} (y_1 - y_2)_t - \Delta(y_1 - y_2) + \epsilon^{-2}(F(y_1) - F(y_2)) &= u_1 - u_2 \\ y_1(0) - y_2(0) &= 0. \end{aligned} \quad (5.10)$$

Rewriting the nonlinear part as

$$\begin{aligned} F(y_1) - F(y_2) &= y_1^3 - y_2^3 - (y_1 - y_2) = (y_1 - y_2)^3 + 3y_1 y_2 (y_1 - y_2) - (y_1 - y_2) \\ &= (y_1 - y_2)^3 + (3y_1^2 - 1)(y_1 - y_2) - 3y_1(y_1 - y_2)^2, \end{aligned}$$

and substituting the above inequality in (5.10), yields

$$\begin{aligned} (y_1 - y_2)_t - \Delta(y_1 - y_2) + \epsilon^{-2}(y_1 - y_2)^3 + \epsilon^{-2}(3y_1^2 - 1)(y_1 - y_2) \\ = u_1 - u_2 + 3\epsilon^{-2} y_1(y_1 - y_2)^2. \end{aligned}$$

Testing against $y_1 - y_2$, gives

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} \|y_1 - y_2\|_{L_2(\Omega)}^2 + \|\nabla(y_1 - y_2)\|_{L_2(\Omega)}^2 + \epsilon^{-2} \|y_1 - y_2\|_{L_4(\Omega)}^4 \\ &+ \epsilon^{-2} (F'(y_1)(y_1 - y_2), y_1 - y_2) \\ &= (u_1 - u_2, y_1 - y_2) + 3\epsilon^{-2} (y_1(y_1 - y_2)^2, y_1 - y_2). \end{aligned} \quad (5.11)$$

Recalling the spectral estimate (3.20) around state solution y_1 with $v = y_1 - y_2 \in H_0^1(\Omega)$, we deduce that

$$\begin{aligned} &\|\nabla(y_1 - y_2)\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(y_1)(y_1 - y_2), y_1 - y_2) \\ &\geq -\lambda(t)(1-\epsilon^2) \|y_1 - y_2\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla(y_1 - y_2)\|_{L_2(\Omega)}^2 \\ &\quad + (F'(y_1)(y_1 - y_2), y_1 - y_2). \end{aligned}$$

Inserting the above estimate into (5.11), using Cauchy-Schwarz and Young inequalities and after standard manipulations we obtain

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} \|y_1 - y_2\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla(y_1 - y_2)\|_{L_2(\Omega)}^2 + \epsilon^{-2} \|y_1 - y_2\|_{L_4(\Omega)}^4 \\ &\leq \frac{1}{2} \|u_1 - u_2\|_{L_2(\Omega)}^2 + (\lambda(t)(1-\epsilon^2) + \frac{3}{2}) \|y_1 - y_2\|_{L_2(\Omega)}^2 \\ &\quad + 3\epsilon^{-2} \|y_1\|_{L_\infty(\Omega)} \|y_1 - y_2\|_{L_3(\Omega)}^3. \end{aligned}$$

Integrating over $t \in (0, \tau)$, we have

$$\begin{aligned} & \| (y_1 - y_2)(\tau) \|_{L_2(\Omega)}^2 + 2\epsilon^2 \int_0^\tau \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}^2 dt + 2\epsilon^{-2} \int_0^\tau \| y_1 - y_2 \|_{L_4(\Omega)}^4 dt \\ & \leq \| (y_1 - y_2)(0) \|_{L_2(\Omega)}^2 + \int_0^\tau \| u_1 - u_2 \|_{L_2(\Omega)}^2 dt + \int_0^\tau \alpha(t) \| y_1 - y_2 \|_{L_2(\Omega)}^2 dt \\ & \quad + 6\epsilon^{-2} \| y_1 \|_{L_\infty(0,T;L_\infty(\Omega))} \int_0^\tau \| y_1 - y_2 \|_{L_3(\Omega)}^3 dt, \end{aligned}$$

where $\alpha(t) = 2\lambda(t)(1 - \epsilon^2) + 3$. The interpolation inequality (5.4), the embedding $H_0^1(\Omega) \subset L_4(\Omega)$ and the Poincaré inequality yield

$$\| y_1 - y_2 \|_{L_3(\Omega)}^3 \leq \frac{C}{\epsilon^2} \| y_1 - y_2 \|_{L_2(\Omega)} \left(\| y_1 - y_2 \|_{L_2(\Omega)}^2 + \epsilon^2 \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}^2 \right),$$

for $C > 0$, depending only on Ω . Then, for $\beta = 1/2$ and

$$\begin{aligned} w_1(\tau) &= \| (y_1 - y_2)(\tau) \|_{L_2(\Omega)}^2, \quad w_2(t) = 2\epsilon^2 \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}^2 + 2\epsilon^{-2} \| y_1 - y_2 \|_{L_4(\Omega)}^4, \\ w_3(t) &= \| y_1 - y_2 \|_{L_3(\Omega)}^3, \quad A = \| u_1 - u_2 \|_{L_2(0,T;L_2(\Omega))}^2, \quad B = 6C\epsilon^{-4} \| y_1 \|_{L_\infty(0,T;L_\infty(\Omega))}, \end{aligned}$$

Lemma 2.5 implies the result for $d = 3$. For $d = 2$, using (5.4) and the GNL inequality (2.3), we deduce,

$$\| y_1 - y_2 \|_{L_3(\Omega)}^3 \leq \tilde{c} \| y_1 - y_2 \|_{L_2(\Omega)}^2 \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}.$$

Therefore, substituting the above inequality and using Young's inequality, we have

$$\begin{aligned} & \| (y_1 - y_2)(\tau) \|_{L_2(\Omega)}^2 + 2\epsilon^2 \int_0^\tau \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}^2 dt + 2\epsilon^{-2} \int_0^\tau \| y_1 - y_2 \|_{L_4(\Omega)}^4 dt \\ & \leq \| (y_1 - y_2)(0) \|_{L_2(\Omega)}^2 + \int_0^\tau \| u_1 - u_2 \|_{L_2(\Omega)}^2 dt + \int_0^\tau \alpha(t) \| y_1 - y_2 \|_{L_2(\Omega)}^2 dt \\ & \quad + 9\tilde{c}^2\epsilon^{-4} \| y_1 \|_{L_\infty(0,T;L_\infty(\Omega))}^2 \int_0^\tau \| y_1 - y_2 \|_{L_2(\Omega)}^2 \| \nabla(y_1 - y_2) \|_{L_2(\Omega)}^2 dt. \end{aligned}$$

The result now follows upon choosing $\beta = 1$, $B = 9\tilde{c}^2\epsilon^{-6} \| y_1 \|_{L_\infty(0,T;L_\infty(\Omega))}^2$ and $\alpha(t) = 2\lambda(t)(1 - \epsilon^2) + 4$ in Lemma 2.5. \square

5.2.2 Differentiability

Next, we determine the first and second order derivatives of G , that play a crucial role in the derivation of the optimality conditions. In this part the analysis of the adjoint state equation is necessary.

Theorem 5.6. Let $u, v \in L_2(0, T; L_2(\Omega))$. The mapping $G : L_2(0, T; L_2(\Omega)) \rightarrow H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$, given by $y_u = G(u)$, is of class C^∞ . Additionally, denoting by $z_v = G'(u)v$ and $z_{vv} = G''(u)v^2$, the latter are the unique solutions to the following problems

$$\begin{aligned} z_{v,t} - \Delta z_v + \epsilon^{-2} (3y_u^2 - 1) z_v &= v \quad \text{in } \Omega_T, \\ z_v &= 0 \quad \text{on } \Sigma_T, \\ z_v(0) &= 0 \quad \text{in } \Omega, \end{aligned} \tag{5.12}$$

$$\begin{aligned} z_{vv,t} - \Delta z_{vv} + \epsilon^{-2} (3y_u^2 - 1) z_{vv} &= -6\epsilon^{-2} y_u z_v^2 \quad \text{in } \Omega_T, \\ z_{vv} &= 0 \quad \text{on } \Sigma_T, \\ z_{vv}(0) &= 0 \quad \text{in } \Omega. \end{aligned} \tag{5.13}$$

Proof. The proof follows using similar arguments as in [CC12, CC16]. Indeed, we consider the mapping

$$F : H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega)) \times L_2(0, T; L_2(\Omega)) \rightarrow L_2(0, T; L_2(\Omega)) \times H_0^1(\Omega),$$

defined through

$$F(y, u) = (y_t - \Delta y + \epsilon^{-2}(y^3 - y) - u, y(0) - y_0).$$

We treat the nonlinear part $d(y) := y^3$ as a Nemytskii operator from $L_6(\Omega_T)$ to $L_2(\Omega_T)$, see, e.g., [Trö10, Section 4.3]. Note that F is of class C^∞ and we have that,

$$\frac{\partial F}{\partial y}(y, u)z = (z_t - \Delta z + \epsilon^{-2}(3y^2 - 1)z, z(0)).$$

We need to ensure that the mapping

$$\frac{\partial F}{\partial y}(y, u) : H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega)) \rightarrow L_2(0, T; L_2(\Omega)) \times H_0^1(\Omega)$$

is an isomorphism from $H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ onto $L_2(0, T; L_2(\Omega)) \times H_0^1(\Omega)$. Indeed, for $y \in H^{2,1}(\Omega_T) \cap L_\infty(0, T; L_\infty(\Omega))$, $f \in L_2(0, T; L_2(\Omega))$ and $z_0 \in H_0^1(\Omega)$ one can prove that z is the unique weak solution of the following linear initial value problem for all $w \in H_0^1(\Omega)$ and for a.e. $t \in (0, T]$

$$\begin{cases} (z_t, w) + (\nabla z, \nabla w) + \epsilon^{-2} ((3y^2 - 1)z, w) = (f, w) \\ z(0) = z_0. \end{cases}$$

through Galerkin method, see [Eva98, Chapter 7]. Furthermore, if y_u is a solution to (5.2) then it holds that $F(y_u, u) = (0, 0)$. The Implicit Function Theorem then implies that the control to state operator, G , is of class C^∞ and, then we can write $F(y_u, u) = F(G(u), u) = (0, 0)$ for all $u \in L_2(0, T; L_2(\Omega))$. The chain rule for all $v \in L_2(0, T; L_2(\Omega))$ yields

$$\frac{\partial F}{\partial y}(y_u, u)G'(u)v + \frac{\partial F}{\partial u}(y_u, u)v = (0, 0),$$

and

$$\begin{aligned} &\frac{\partial^2 F}{\partial y^2}(y_u, u)(G'(u)v, G'(u)v) + \frac{\partial F}{\partial y}(y_u, u) G''(u)v^2 \\ &+ 2 \frac{\partial F}{\partial u \partial y}(y_u, u)(G'(u)v, v) + \frac{\partial^2 F}{\partial u^2}(y_u, u) v^2 = (0, 0). \end{aligned}$$

Upon setting $z_v = G'(u)v$ and $z_{vv} = G''(u)v^2$, the equations (5.12) and (5.13) are shown, respectively. \square

The above differentiability properties of G imply that the reduced cost functional $J : L_2(0, T; L_2(\Omega)) \rightarrow \mathbb{R}$ is of class C^∞ , also.

Lemma 5.7. For any $u, v \in L_2(0, T; L_2(\Omega))$ and $\mu > 0$ it holds that

$$J'(u)v = \int_0^T \int_{\Omega} (\varphi_u + \mu u)v \, dx \, dt, \quad (5.14)$$

and

$$\begin{aligned} J''(u)v^2 &= \int_0^T \int_{\Omega} |z_v|^2 \, dx \, dt + \gamma \int_{\Omega} |z_v(T)|^2 \, dx + \mu \int_0^T \int_{\Omega} |v|^2 \, dx \, dt \\ &\quad - 6\epsilon^{-2} \int_0^T \int_{\Omega} y_u z_v^2 \varphi_u \, dx \, dt, \end{aligned} \quad (5.15)$$

where z_v is the solution of (5.12) and $\varphi_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ is the unique solution that satisfies the adjoint state problem,

$$\begin{cases} -(\varphi_{u,t}, w) + (\nabla \varphi_u, \nabla w) + \epsilon^{-2}((3y_u^2 - 1)\varphi_u, w) = (y_u - y_d, w), \\ \varphi_u(T) = \gamma(y_u(T) - y_\Omega), \end{cases} \quad (5.16)$$

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

Proof. To begin with, the derivation of the adjoint state equation results through a standard Lagrangian method, see [Trö10, Chapter 3]. Then, after standard argumentation we conclude that (5.16) admits a unique weak solution with desirable regularity. Using the chain rule, we immediately deduce that

$$\begin{aligned} J'(u)v &= \int_0^T \int_{\Omega} (y_u - y_d)z_v \, dx \, dt + \gamma \int_{\Omega} (y_u(T) - y_\Omega)z_v(T) \, dx \\ &\quad + \mu \int_0^T \int_{\Omega} uv \, dx \, dt. \end{aligned}$$

We will eliminate z_v using the adjoint problem. Specifically, testing (5.16) against z_v and (5.12) against φ_u , integrating by parts with respect to time variable from 0 up to T , and using the resulting equations, we obtain

$$\int_0^T (\varphi_u, v) \, dt = \gamma (y_u(T) - y_\Omega, z_v(T)) + \int_0^T (y_u - y_d, z_v) \, dt.$$

Combining the last two equations, we deduce (5.14).

We continue with the proof of (5.15). Using the product rule, we have

$$\begin{aligned} J''(u)v^2 &= \int_0^T \int_{\Omega} |z_v|^2 \, dx \, dt + \int_0^T \int_{\Omega} (y_u - y_d)z_{vv} \, dx \, dt + \gamma \int_{\Omega} |z_v(T)|^2 \, dx \\ &\quad + \gamma \int_{\Omega} (y_u(T) - y_\Omega)z_{vv}(T) \, dx + \mu \int_0^T \int_{\Omega} |v|^2 \, dx \, dt. \end{aligned}$$

Testing (5.16) against z_{vv} , integrating in space-time and substituting the conditions $z_{vv}(0) = 0$ and $\varphi_u(T) = \gamma(y_u(T) - y_\Omega)$, yields

$$\begin{aligned} &\int_0^T (\varphi_u, z_{vv,t}) + (\nabla \varphi_u, \nabla z_{vv}) + \epsilon^{-2}((3y_u^2 - 1)\varphi_u, z_{vv}) \, dt \\ &= \gamma (y_u(T) - y_\Omega, z_{vv}(T)) + \int_0^T (y_u - y_d, z_{vv}) \, dt. \end{aligned} \quad (5.17)$$

Then, testing (5.13) against φ_u and working analogously, we get that

$$\begin{aligned} & \int_0^T (z_{vv,t}, \varphi_u) + (\nabla z_{vv}, \nabla \varphi_u) + \epsilon^{-2} ((3y_u^2 - 1)z_{vv}, \varphi_u) dt \\ &= -6\epsilon^{-2} \int_0^T (y_u z_v^2, \varphi_u) dt. \end{aligned} \quad (5.18)$$

We observe that (5.17) and (5.18) imply

$$\int_0^T (y_u - y_d, z_{vv}) dt + \gamma (y_u(T) - y_\Omega, z_{vv}(T)) = -6\epsilon^{-2} \int_0^T (y_u z_v^2, \varphi_u) dt,$$

which completes the proof. \square

Remark 5.8. The assumption $y_\Omega \in H_0^1(\Omega)$, together with the regularity properties of the state solution y_u , implies that $\varphi_u(T) \in H_0^1(\Omega)$. Thus, we deduce that

$$\|\varphi_u(T)\|_{H_0^1(\Omega)} = \|\gamma(y_u(T) - y_\Omega)\|_{H_0^1(\Omega)} \leq \gamma \left(\sup_{t \in [0, T]} \|y_u(t)\|_{H_0^1(\Omega)} + \|y_\Omega\|_{H_0^1(\Omega)} \right).$$

Recalling Lemma 5.1 and the embedding $H^{2,1}(\Omega_T) \subset C(0, T; H^1(\Omega))$, we obtain

$$\|\varphi_u(T)\|_{H_0^1(\Omega)} \leq C\epsilon^{-2} \quad \text{when} \quad \epsilon \|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq C.$$

Similarly, we have that

$$\|\varphi_u(T)\|_{H_0^1(\Omega)} \leq C\epsilon^{-1} \quad \text{when} \quad \|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq D.$$

Lemma 5.9. Let φ_u be the solution to (5.16), $y_d \in L_2(0, T; L_2(\Omega))$ and $y_\Omega \in H_0^1(\Omega)$. Then, there exists a constant $C > 0$, depending only on the domain Ω such that

$$\begin{aligned} & \sup_{t \in [0, T]} \|\varphi_u(t)\|_{L_2(\Omega)} + \epsilon \|\nabla \varphi_u\|_{L_2(0, T; L_2(\Omega))} + \|\varphi_u y_u\|_{L_2(0, T; L_2(\Omega))} \\ & \leq CC_\varphi^{1/2} \left(\|\varphi_u(T)\|_{L_2(\Omega)} + \|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} \right) := D_{st,1}, \end{aligned} \quad (5.19)$$

$$\begin{aligned} & \|\varphi_{u,t}\|_{L_2(0, T; L_2(\Omega))} + \sup_{t \in [0, T]} \|\nabla \varphi_u(t)\|_{L_2(\Omega)} \\ & \leq C \left(\|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} + \frac{1}{\epsilon^2} \left(\|y_u\|_{L_\infty(0, T; L_\infty(\Omega))} + T^{1/2} D_{st,1} \right) \right. \\ & \quad \left. + \|\nabla \varphi_u(T)\|_{L_2(\Omega)} \right) := D_{st,2}, \end{aligned} \quad (5.20)$$

$$\|\varphi_u\|_{L_2(0, T; H^2(\Omega))} \quad (5.21)$$

$$\leq C \left(\|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} + D_{st,2} + \frac{1}{\epsilon^2} (1 + 3\|y_u\|_{L_\infty(0, T; L_\infty(\Omega))}) D_{st,1} \right),$$

where $C_\varphi := \exp \left(\int_0^T (2\lambda(t)(1 - \epsilon^2) + 3) dt \right)$.

Proof. To derive the first stability estimate, we test (5.16) against $w = \varphi_u$, to obtain

$$-\frac{1}{2} \frac{d}{dt} \|\varphi_u\|_{L_2(\Omega)}^2 + \|\nabla \varphi_u\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(y_u) \varphi_u, \varphi_u) = (y_u - y_d, \varphi_u).$$

Using (3.20) for $v = \varphi_u$ about state solution y_u , applying Cauchy-Schwarz and Young's inequalities on the right-hand side and integrating with respect to $t \in (\tau, T)$, we obtain

$$\begin{aligned} & \|\varphi_u(\tau)\|_{L_2(\Omega)}^2 + 2\epsilon^2 \int_\tau^T \|\nabla \varphi_u\|_{L_2(\Omega)}^2 dt + 6 \int_\tau^T \|\varphi_u y_u\|_{L_2(\Omega)}^2 dt \\ & \leq \|\varphi_u(T)\|_{L_2(\Omega)}^2 + \int_\tau^T (2\lambda(t)(1-\epsilon^2)+3) \|\varphi_u\|_{L_2(\Omega)}^2 dt + \int_\tau^T \|y_u - y_d\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

The (linear) Gronwall inequality yields (5.19).

Setting $w = -\varphi_{u,t}$ into (5.16), gives

$$\|\varphi_{u,t}\|_{L_2(\Omega)}^2 - \frac{1}{2} \frac{d}{dt} \|\nabla \varphi_u\|_{L_2(\Omega)}^2 = (y_u - y_d, \varphi_{u,t}) + \epsilon^{-2} (F'(y_u) \varphi_u, \varphi_{u,t}).$$

Now using Young's inequality, we may bound the last two terms on the right-hand side as follows:

$$\begin{aligned} \epsilon^{-2} |(F'(y_u) \varphi_u, \varphi_{u,t})| &= \epsilon^{-2} |((3y_u^2 - 1)\varphi_u, \varphi_{u,t})| \\ &\leq \frac{1}{4} \|\varphi_{u,t}\|_{L_2(\Omega)}^2 + 18\epsilon^{-4} \|y_u\|_{L_\infty(\Omega)}^2 \|\varphi_u y_u\|_{L_2(\Omega)}^2 + 2\epsilon^{-4} \|\phi_u\|_{L_2(\Omega)}^2, \end{aligned}$$

and

$$|(y_u - y_d, \varphi_{u,t})| \leq \frac{1}{4} \|\varphi_{u,t}\|_{L_2(\Omega)}^2 + \|y_u - y_d\|_{L_2(\Omega)}^2.$$

Substituting the last two inequalities and integrating from τ up to T yields,

$$\begin{aligned} & \int_\tau^T \|\varphi_{u,t}\|_{L_2(\Omega)}^2 dt + \|\nabla \varphi_u(\tau)\|_{L_2(\Omega)}^2 \\ & \leq 2 \int_\tau^T \|y_u - y_d\|_{L_2(\Omega)}^2 dt + \|\nabla \varphi_u(T)\|_{L_2(\Omega)}^2 + 4\epsilon^{-4} \int_\tau^T \|\varphi_u\|_{L_2(\Omega)}^2 dt \\ & \quad + 36\epsilon^{-4} \|y_u\|_{L_\infty(0,T;L_\infty(\Omega))}^2 \int_\tau^T \|\varphi_u y_u\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

Using now the stability bound (5.19), we obtain (5.20). The third estimate follows using similar techniques by setting $w = -\Delta \varphi_u$ into (5.16) and using the previous bounds to estimate $\|\varphi_{u,t}\|_{L_2(0,T;L_2(\Omega))}$, $\|\nabla \varphi_u\|_{L_2(0,T;L_2(\Omega))}$ and $\|y_u \varphi_u\|_{L_2(0,T;L_2(\Omega))}$. \square

Let $u_1, u_2 \in L_2(0, T; L_2(\Omega))$ be the control functions. Then, we denote by $y_i = y_{u_i}$ and $\varphi_i = \varphi_{u_i}$ the associated state and adjoint state solutions for $i = 1, 2$, respectively.

Lemma 5.10. Assume that (5.8) holds. Then, for $d = 2$, there exists a constant $C_T > 0$ depending only on the domain Ω_T , such that

$$\begin{aligned} & \sup_{t \in [0, T]} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)} + \epsilon \|\varphi_1 - \varphi_2\|_{L_2(0, T; H_0^1(\Omega))} \\ & \leq C_T E_\varphi^{1/2} L_1 \left(1 + \frac{C_\infty \tilde{c} D_{st,1}}{\epsilon^{7/2}} \right) \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))}. \end{aligned} \tag{5.22}$$

For $d = 3$, there exists a constant $C_T > 0$ depending only on the domain Ω_T , such that

$$\begin{aligned} & \sup_{t \in [0, T]} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)} + \epsilon \|\varphi_1 - \varphi_2\|_{L_2(0, T; H_0^1(\Omega))} \\ & \leq C_T E_\varphi^{1/2} L_1 \left(1 + \frac{C_\infty \tilde{c} D_{st,1}}{\epsilon^{15/4}} \right) \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))}, \end{aligned} \quad (5.23)$$

where $C_\infty := \left(C (\|y_1\|_{L_\infty(0, T; L_\infty(\Omega))}^2 + \|y_2\|_{L_\infty(0, T; L_\infty(\Omega))}^2) \right)^{1/2}$ with $C > 0$ depending on $|\Omega|$, and $E_\varphi := \int_0^T (2\lambda(t)(1 - \epsilon^2) + 4) dt$.

Proof. Subtracting the equations satisfied by φ_1 and φ_2 , it yields that

$$\begin{cases} -(\varphi_1 - \varphi_2)_t - \Delta(\varphi_1 - \varphi_2) + \epsilon^{-2} (F'(y_1)\varphi_1 - F'(y_2)\varphi_2) = y_1 - y_2 \\ (\varphi_1 - \varphi_2)(T) = \gamma(y_1 - y_2)(T). \end{cases} \quad (5.24)$$

Inserting the identity

$$F'(y_1)\varphi_1 - F'(y_2)\varphi_2 = (3y_1^2 - 1)(\varphi_1 - \varphi_2) + 3(y_1^2 - y_2^2)\varphi_2,$$

into (5.24) and testing against $\varphi_1 - \varphi_2$, we deduce that

$$\begin{aligned} & -\frac{1}{2} \frac{d}{dt} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)}^2 + \|\nabla(\varphi_1 - \varphi_2)\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(y_1)(\varphi_1 - \varphi_2), \varphi_1 - \varphi_2) \\ & = (y_1 - y_2, \varphi_1 - \varphi_2) - 3\epsilon^{-2} ((y_1^2 - y_2^2)\varphi_2, \varphi_1 - \varphi_2) := \mathcal{K}_1 + \mathcal{K}_2. \end{aligned}$$

We have

$$\mathcal{K}_1 \leq \frac{1}{2} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)}^2 + \frac{1}{2} \|y_1 - y_2\|_{L_2(\Omega)}^2,$$

while applying Hölder, Poincaré and Young inequalities, we obtain

$$\begin{aligned} \mathcal{K}_2 & \leq 3\epsilon^{-2} \|y_1 - y_2\|_{L_2(\Omega)} \left(\|y_1\|_{L_\infty(\Omega)} + \|y_2\|_{L_\infty(\Omega)} \right) \|\varphi_2\|_{L_4(\Omega)} \|\varphi_1 - \varphi_2\|_{L_4(\Omega)} \\ & \leq \frac{C_\infty}{\epsilon^6} \|y_1 - y_2\|_{L_2(\Omega)}^2 \|\varphi_2\|_{L_4(\Omega)}^2 + \frac{\epsilon^2}{2} \|\nabla(\varphi_1 - \varphi_2)\|_{L_2(\Omega)}^2. \end{aligned}$$

Collecting the above bounds and using (3.20) for $v = \varphi_1 - \varphi_2$, $y = y_1$, and integrating with respect to $t \in (\tau, T)$, results into

$$\begin{aligned} & \|(\varphi_1 - \varphi_2)(\tau)\|_{L_2(\Omega)}^2 + \epsilon^2 \int_\tau^T \|\nabla(\varphi_1 - \varphi_2)\|_{L_2(\Omega)}^2 dt \\ & \leq \|\gamma(y_1 - y_2)(T)\|_{L_2(\Omega)}^2 + \frac{C_\infty^2}{\epsilon^6} \|y_1 - y_2\|_{L_\infty(0, T; L_2(\Omega))}^2 \int_\tau^T \|\varphi_2\|_{L_4(\Omega)}^2 dt \\ & \quad + \int_\tau^T \|y_1 - y_2\|_{L_2(\Omega)}^2 dt + \int_\tau^T (2\lambda(t)(1 - \epsilon^2) + 4) \|\varphi_1 - \varphi_2\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

For $d = 3$, using the GNL inequality, Hölder's inequality with $s_1 = 4$ and $s_2 = 4/3$, and (5.19), we estimate

$$\begin{aligned} \int_\tau^T \|\varphi_2\|_{L_4(\Omega)}^2 dt & \leq \tilde{c}^2 \int_\tau^T \|\varphi_2\|_{L_2(\Omega)}^{1/2} \|\nabla \varphi_2\|_{L_2(\Omega)}^{3/2} dt \\ & \leq \tilde{c}^2 \|\varphi_2\|_{L_2(0, T; L_2(\Omega))}^{1/2} \|\nabla \varphi_2\|_{L_2(0, T; L_2(\Omega))}^{3/2} \leq T^{1/4} \frac{\tilde{c}^2 D_{st,1}^2}{\epsilon^{3/2}}. \end{aligned}$$

Similarly, for $d = 2$, we have

$$\begin{aligned} \int_{\tau}^T \|\varphi_2\|_{L_4(\Omega)}^2 dt &\leq \tilde{c}^2 \int_{\tau}^T \|\varphi_2\|_{L_2(\Omega)} \|\nabla \varphi\|_{L_2(\Omega)} dt \\ &\leq \tilde{c}^2 \|\varphi_2\|_{L_2(0,T;L_2(\Omega))} \|\nabla \varphi_2\|_{L_2(0,T;L_2(\Omega))} \leq T^{1/2} \frac{\tilde{c}^2 D_{st,1}^2}{\epsilon}. \end{aligned}$$

Then, for $d = 3$, the (linear) Gronwall inequality implies

$$\begin{aligned} &\sup_{t \in [0,T]} \|(\varphi_1 - \varphi_2)(t)\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla(\varphi_1 - \varphi_2)\|_{L_2(0,T;L_2(\Omega))}^2 \\ &\leq E_{\varphi} \left(\|\gamma(y_1 - y_2)(T)\|_{L_2(\Omega)}^2 + \left(T + \frac{T^{1/4} C_{\infty}^2 D_{st,1}^2}{\epsilon^{15/2}} \right) \sup_{t \in [0,T]} \|y_1 - y_2\|_{L_2(\Omega)}^2 \right). \end{aligned}$$

The estimate now follows by recalling the Lipschitz continuity of control to state operator from $L_2(0, T; L_2(\Omega))$ into $L_{\infty}(0, T; L_2(\Omega))$. Working in a completely analogous fashion, we deduce the estimate for $d = 2$. \square

5.2.3 Necessary and sufficient conditions

Below, we state the optimality conditions. We refer the readers to [CC12, Theorems 3.4 and 3.3] for the related proofs.

Theorem 5.11. Every locally optimal control \bar{u} for problem (5.3), satisfies, together with its associated state $\bar{y} \in H^{2,1}(\Omega_T)$ and adjoint state $\bar{\varphi} \in H^{2,1}(\Omega_T)$

$$\begin{cases} (\bar{y}_t, v) + (\nabla \bar{y}, \nabla v) + \epsilon^{-2} (\bar{y}^3 - \bar{y}, v) = (\bar{u}, v) \quad \forall v \in H_0^1(\Omega) \\ \bar{y}(0) = y_0, \end{cases} \quad (5.25)$$

$$\begin{cases} -(\bar{\varphi}_t, w) + (\nabla \bar{\varphi}, \nabla w) + \epsilon^{-2} ((3\bar{y}^2 - 1) \bar{\varphi}, w) = (\bar{y} - y_d, w) \quad \forall w \in H_0^1(\Omega) \\ \bar{\varphi}(T) = \gamma(\bar{y}(T) - y_{\Omega}), \end{cases} \quad (5.26)$$

and the variational inequality (optimality condition)

$$\int_0^T \int_{\Omega} (\bar{\varphi} + \mu \bar{u}) (u - \bar{u}) dx dt \geq 0 \quad \forall u \in U_{ad}, \quad (5.27)$$

with $\bar{u} \in C(0, T; H^1(\Omega)) \cap H^1(\Omega_T)$.

Furthermore, assume that $\epsilon \|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq C$. Then,

$$\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C} \epsilon^{-2} \text{ and } \|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D} \epsilon^{-3}.$$

If in addition $\|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq D$, then

$$\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C} \epsilon^{-1} \text{ and } \|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D} \epsilon^{-2};$$

here, the constants \tilde{C}, \tilde{D} are independent of ϵ and depend only on the data.

Proof. Note that every local optimal solution satisfies $J'(\bar{u})(u - \bar{u}) \geq 0, \forall u \in U_{ad}$. Indeed, let $u \in U_{ad}$ be arbitrary. Since U_{ad} is convex, $\bar{u} + \rho(u - \bar{u}) \in U_{ad}$ for any $\rho \in (0, 1]$. Since \bar{u} is an optimal solution, it yields that

$$J(\bar{u} + \rho(u - \bar{u})) \geq J(\bar{u}).$$

Hence, for $\rho \in (0, 1]$ we have that

$$\frac{1}{\rho} (J(\bar{u} + \rho(u - \bar{u})) - J(\bar{u})) \geq 0.$$

Letting $\rho \rightarrow 0$, we arrive at $J'(\bar{u})(u - \bar{u}) \geq 0$, which proves the validity of (5.27). Then, it is enough to recall the derivative expression (5.14) to derive the optimality system (5.25)-(5.26) and (5.27). Inequality (5.27) implies the standard projection formula

$$\bar{u}(t, x) = \text{Proj}_{[u_a, u_b]} \left(-\frac{1}{\mu} \bar{\varphi}(t, x) \right) \text{ for a.e. } (t, x) \in \Omega_T, \quad (5.28)$$

from which we deduce $\bar{u} \in H^1(\Omega_T) \cap C(0, T; H^1(\Omega))$. Here, for real numbers $u_a \leq u_b$, we denote by $\text{Proj}_{[u_a, u_b]}$ the projection of \mathbb{R} onto $[u_a, u_b]$,

$$\text{Proj}_{[u_a, u_b]}(u) := \min \{u_b, \max\{u_a, u\}\}.$$

Therefore, if

$$\epsilon \|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2} \|(y_0^2 - 1)^2\|_{L^1(\Omega)}^{1/2} \leq C,$$

(independent of ϵ) we observe that the constants $C_{st,2}, C_{st,3}$ of Lemma 5.1 satisfy

$$C_{st,2} \leq \left(\frac{C}{\epsilon} + \|\bar{u}\|_{L_2(0,T;L_2(\Omega))} \right) \quad \text{and} \quad C_{st,3} \leq \left(\frac{C}{\epsilon^2} + \|\bar{u}\|_{L_2(0,T;L_2(\Omega))} \right)$$

from which we deduce that $\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C}\epsilon^{-2}$. Similar, the estimates of Lemma 5.9, imply that $\|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D}\epsilon^{-3}$ when $\gamma > 0$ and $\|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D}\epsilon^{-2}$ when $\gamma = 0$. Under the assumption

$$\|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L^1(\Omega)}^{1/2} \leq D,$$

a similar boot-strap argument, imply that $\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C}\epsilon^{-1}$ and $\|\bar{\phi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D}\epsilon^{-2}$. We note here that Lemma 5.1 implies that the constant $D_{st,1}$ of (5.19) is bounded independently of ϵ . \square

In the usual manner, we deduce from (5.27) that for a.e. $(t, x) \in \Omega_T$,

$$\begin{cases} \bar{u}(t, x) = u_a \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \geq 0, \\ \bar{u}(t, x) = u_b \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \leq 0, \\ \bar{u}(t, x) \in (u_a, u_b) \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) = 0, \end{cases} \quad (5.29)$$

and

$$\begin{cases} \bar{\varphi}(t, x) + \mu \bar{u}(t, x) > 0 \Rightarrow \bar{u}(t, x) = u_a, \\ \bar{\varphi}(t, x) + \mu \bar{u}(t, x) < 0 \Rightarrow \bar{u}(t, x) = u_b. \end{cases} \quad (5.30)$$

We introduce the cone of critical directions that is necessary to state the second order conditions:

$$\mathcal{C}_{\bar{u}} := \{v \in L_2(0, T; L_2(\Omega)) : v \text{ satisfies (5.32)}\}, \quad (5.31)$$

where

$$\begin{cases} i) & v(t, x) = 0 \quad \text{if } \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \neq 0, \\ ii) & v(t, x) \geq 0 \quad \text{if } \bar{u}(t, x) = u_a, \\ iii) & v(t, x) \leq 0 \quad \text{if } \bar{u}(t, x) = u_b. \end{cases} \quad (5.32)$$

Let us notice that

$$\begin{aligned} J'(\bar{u})v &= \int_0^T \int_{\Omega} (\bar{\varphi}(t, x) + \mu \bar{u}(t, x)) v(t, x) \, dx \, dt, \\ (\bar{\varphi}(t, x) + \mu \bar{u}(t, x)) v(t, x) &= 0 \text{ for a.e. } (t, x) \in \Omega_T \text{ and for every } v \in \mathcal{C}_{\bar{u}}. \end{aligned} \quad (5.33)$$

Theorem 5.12. Let \bar{u} be a local solution of the problem (5.3). Then, it holds that

$$J''(\bar{u})v^2 \geq 0 \quad \forall v \in \mathcal{C}_{\bar{u}}. \quad (5.34)$$

Proof. The proof follows completely analogously to [CC12, CC16]. Let $v \in \mathcal{C}_{\bar{u}}$ be arbitrary and let $r < (u_b - u_a)/2$ that defines

$$v_r(t, x) = \begin{cases} 0 & \text{if } u_a < \bar{u}(t, x) < u_a + r, \\ 0 & \text{if } u_b - r < \bar{u}(t, x) < u_b, \\ \text{Proj}_{[-1/r, 1/r]} v(t, x) & \text{otherwise.} \end{cases}$$

We can check that $v_r \in \mathcal{C}_{\bar{u}}$ for every $r > 0$. We observe that $v_r(t, x) \rightarrow v(t, x)$ pointwise a.e. as $r \rightarrow 0$. Also, $v_r^2(t, x) \leq v^2(t, x)$ for a.e. (t, x) and for every $r > 0$. Then, we may use Lebesgue's dominated convergence theorem to deduce that $v_r \rightarrow v$ strongly in $L_2(0, T; L_2(\Omega))$.

Moreover, $\bar{u} + \rho v_r \in U_{ad}$ for $0 < \rho < r^2$. We make a second order Taylor expansion of J at \bar{u} for some $0 < \theta_\rho < \rho$ such that

$$0 \leq J(\bar{u} + \rho v_r) - J(\bar{u}) = \rho J'(\bar{u})v_r + \frac{\rho^2}{2} J''(\bar{u} + \theta_\rho v_r) v_r^2,$$

at the first step we took into account the fact that \bar{u} is a local minimum. The observation $v_r \in \mathcal{C}_{\bar{u}}$ implies that $J'(\bar{u})v_r = 0$ according to (5.33). Hence, the above inequality leads to $J''(\bar{u} + \theta_\rho v_r) v_r^2 \geq 0$.

Next, we take the limit as $\rho \rightarrow 0$ ($\theta_\rho \rightarrow 0$) to get $J''(\bar{u})v^2 \geq 0$. Now through the definition of $J''(u)$, we obtain that

$$\begin{aligned} J''(\bar{u})v_r^2 &= \int_0^T \int_{\Omega} |z_{v_r}|^2 \, dx \, dt + \gamma \int_{\Omega} |z_{v_r}(T)|^2 \, dx + \mu \int_0^T \int_{\Omega} |v_r|^2 \, dx \, dt \\ &\quad - 6\epsilon^{-2} \int_0^T \int_{\Omega} y_{\bar{u}} z_{v_r}^2 \varphi_{\bar{u}} \, dx \, dt \\ &\longrightarrow \int_0^T \int_{\Omega} |z_v|^2 \, dx \, dt + \gamma \int_{\Omega} |z_v(T)|^2 \, dx + \mu \int_0^T \int_{\Omega} |v|^2 \, dx \, dt \\ &\quad - 6\epsilon^{-2} \int_0^T \int_{\Omega} y_{\bar{u}} z_v^2 \varphi_{\bar{u}} \, dx \, dt = J''(\bar{u})v^2, \end{aligned}$$

as taking the limit $r \rightarrow 0$. To pass the limit, we note that since $v_r \rightarrow v$ strongly in $L_2(0, T; L_2(\Omega))$, using the definition of z_v, z_{v_r} through (5.12) we also deduce that $z_{v_r} \rightarrow z_v$ in $L_2(0, T; H^1(\Omega)) \cap L_\infty(0, T; L_2(\Omega))$. \square

Now, we shall state the sufficient conditions for optimality.

Theorem 5.13. Assume that $\bar{u} \in U_{ad}$ satisfies

$$J'(\bar{u})(u - \bar{u}) \geq 0 \quad \forall u \in U_{ad}, \quad (5.35)$$

$$J''(\bar{u})v^2 > 0 \quad \forall v \in \mathcal{C}_{\bar{u}} \setminus \{0\}. \quad (5.36)$$

Then, there exist $\alpha > 0$ and $\delta > 0$, such that

$$J(\bar{u}) + \frac{\delta}{2} \|u - \bar{u}\|_{L_2(0, T; L_2(\Omega))}^2 \leq J(u) \quad \forall u \in U_{ad} \cap B_\alpha(\bar{u}), \quad (5.37)$$

where $B_\alpha(\bar{u})$ is the open ball of $L_2(0, T; L_2(\Omega))$ centered at \bar{u} with radius α .

Proof. The proof follows completely analogously to [CC12, CC16] based on arguments of [CMR07] (see also references within). We note that $\|y_u\|_{L_2(0, T; L_2(\Omega))}$ is bounded independently of ϵ , for any $u \in U_{ad}$; see Lemma 5.1.

The proof follows by contradiction. Indeed, let us suppose that the theorem is false. Then, there exists a sequence $\{u_k\}_{k=1}^\infty \subset U_{ad}$ such that

$$\|\bar{u} - u_k\|_{L_2(0, T; L_2(\Omega))} \leq \frac{1}{k} \text{ and } J(\bar{u}) + \frac{1}{2k} \|\bar{u} - u_k\|_{L_2(0, T; L_2(\Omega))}^2 > J(u_k). \quad (5.38)$$

Now, we define

$$\rho_k = \|\bar{u} - u_k\|_{L_2(0, T; L_2(\Omega))} \quad \text{and} \quad v_k = \frac{1}{\rho_k} (u_k - \bar{u}). \quad (5.39)$$

Then, taking a subsequence if necessary, we can assume that $v_k \rightharpoonup v$ weakly in $L_2(0, T; L_2(\Omega))$. The proof is divided into three steps.

Step I: $v \in \mathcal{C}_{\bar{u}}$. We have to prove that v satisfies (5.32). First, we observe that the set of elements in $L_2(0, T; L_2(\Omega))$ satisfying *ii*) – *iii*) of (5.32) is closed and convex. From the definition of v_k , it is obvious that each v_k satisfies *ii*) – *iii*) of (5.32). Let us prove *i*). From (5.38) and using mean value theorem we get for some $0 < \theta_k < 1$ that

$$\begin{aligned} J(\bar{u}) + \frac{1}{2k} \|\bar{u} - u_k\|_{L_2(0, T; L_2(\Omega))}^2 &= J(\bar{u}) + \frac{\rho_k^2}{2k} > J(u_k) = J(\bar{u} + \rho_k v_k) \\ &= J(\bar{u}) + \rho_k J'(\bar{u} + \theta_k \rho_k v_k) v_k, \end{aligned}$$

hence

$$J'(\bar{u} + \theta_k \rho_k v_k) v_k < \frac{\rho_k}{2k} \rightarrow 0. \quad (5.40)$$

Let us prove that $J'(\bar{u} + \theta_k \rho_k v_k) v_k \rightarrow J'(\bar{u})v$. To this end, we set $u_{\theta_k} = \bar{u} + \theta_k \rho_k v_k$. From, (5.38) and (5.39) we know that $u_{\theta_k} \rightarrow \bar{u}$ in $L_2(0, T; L_2(\Omega))$ strongly. Therefore, its associated state y_{θ_k} and adjoint state φ_{θ_k} converge strongly to \bar{y} and $\bar{\varphi}$ in $H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$, then with (5.14) we have that

$$\begin{aligned} J'(\bar{u} + \theta_k \rho_k v_k) v_k &= \int_0^T \int_\Omega \left(\varphi_{\theta_k} + \mu u_{\theta_k} \right) v_k \, dx \, dt \\ &\rightarrow \int_0^T \int_\Omega (\bar{\varphi} + \mu \bar{u}) v \, dx \, dt = J'(\bar{u})v. \end{aligned}$$

Then, (5.40) implies that $J'(\bar{u})v \leq 0$. Note that since (5.35) holds, then (5.29) holds as well. So far we know that v satisfies $ii) - iii)$ of (5.32). Thus, almost for every $(t, x) \in \Omega_T$ we have that $(\bar{\varphi}(t, x) + \mu\bar{u}(t, x)) v(t, x) \geq 0$, that together with $J'(\bar{u})v \leq 0$ yield that v satisfies $i)$ of (5.32).

Step II: $v = 0$. We will prove that $J''(\bar{u})v^2 \leq 0$, then according to the second assumption of the theorem this is possible only if $v = 0$. Using again (5.38), (5.39) and making use of Taylor expansion, we get for some $0 < \theta_k < 1$

$$\begin{aligned} J(\bar{u}) + \frac{\rho_k^2}{2k} &> J(u_k) = J(\bar{u} + \rho_k v_k) \\ &= J(\bar{u}) + \rho_k J'(\bar{u})v_k + \frac{\rho_k^2}{2} J''(\bar{u} + \theta_k \rho_k v_k)v_k^2, \end{aligned}$$

hence since $\rho_k J'(\bar{u})v_k = J'(\bar{u})(u_k - \bar{u}) \geq 0$ we get that

$$J''(\bar{u} + \theta_k \rho_k v_k)v_k^2 < \frac{1}{k}. \quad (5.41)$$

Now, we set $u_{\theta_k} = \bar{u} + \theta_k \rho_k v_k$ where $u_{\theta_k} \rightarrow \bar{u}$ in $L_2(0, T; L_2(\Omega))$ strongly. Then, $y_{\theta_k} = G(u_{\theta_k})$ and φ_{θ_k} the corresponding state and adjoint state, respectively. We also denote $z_{\theta_k} = G'(u_{\theta_k})v_k$ and from (5.15) we have that

$$\begin{aligned} J''(u_{\theta_k})v_k^2 &= \int_0^T \int_{\Omega} |z_{\theta_k}|^2 dx dt + \gamma \int_{\Omega} |z_{\theta_k}(T)|^2 dx + \mu \int_0^T \int_{\Omega} |v_k|^2 dx dt \\ &\quad - 6\epsilon^{-2} \int_0^T \int_{\Omega} y_{\theta_k} z_{\theta_k}^2 \varphi_{\theta_k} dx dt. \end{aligned} \quad (5.42)$$

It is easy to pass the limit since $z_{\theta_k} \rightharpoonup z_v$ weakly in $H^{2,1}(\Omega_T)$ while $y_{\theta_k} \rightarrow \bar{y}$ and $\varphi_{\theta_k} \rightarrow \bar{\varphi}$ strongly in $H^{2,1}(\Omega_T)$. In the third integral we use the weakly lower semi-continuity in $L_2(0, T; L_2(\Omega))$. Thus, we deduce from (5.41) and (5.42)

$$J''(\bar{u})v^2 \leq \liminf_{k \rightarrow \infty} J''(u_{\theta_k})v_k^2 \leq 0. \quad (5.43)$$

Step III: Final contradiction. Since $v = 0$ we get that $z_{\theta_k} \rightharpoonup 0$ weakly in $H^{2,1}(\Omega_T)$. Then, from (5.42) and (5.43) together with the identity $\|v_k\|_{L_2(0, T; L_2(\Omega))} = 1$ allow us to conclude that

$$0 \geq \liminf_{k \rightarrow \infty} J''(u_{\theta_k})v_k^2 = 0 + \mu = \mu,$$

which is a contradiction. \square

We point out that the constant $\delta > 0$ will not appear on any exponent, in what follows.

Remark 5.14. The second order sufficient condition (5.36) is equivalent to

$$J''(\bar{u})v^2 \geq \delta \|v\|_{L_2(0, T; L_2(\Omega))}^2 \quad \forall v \in \mathcal{C}_{\bar{u}}. \quad (5.44)$$

Indeed, let us observe that (5.37) implies that \bar{u} is a local optimal solution to the problem

$$\begin{cases} \min J_{\delta}(u) = J(u) - \frac{\delta}{2} \|u - \bar{u}\|_{L_2(0, T; L_2(\Omega))}^2 \\ u \in U_{ad} \cap B_{\alpha}(\bar{u}). \end{cases} \quad (5.45)$$

Then, Theorem 5.12 yields that $J''_{\delta}(\bar{u})v^2 \geq 0$ for all $v \in \mathcal{C}_{\bar{u}}$. Thus, we deduce

$$J''_{\delta}(\bar{u})v^2 = J''(\bar{u})v^2 - \delta\|v\|_{L_2(0,T;L_2(\Omega))}^2 \geq 0,$$

which implies the assertion.

CHAPTER 6

APPROXIMATION OF THE CONTROL PROBLEM

This chapter is devoted to the numerical approximation of the optimal control problem. We shall present *a priori* error estimates for a fully-discrete scheme based on the discontinuous-in time-Galerkin dG(0) framework, i.e. piece-wise constant approximations in time, finite elements based on piecewise linear polynomials approximations in space. The numerical analysis of the control to state under low regularity assumptions is based on the construction of a globally space-time projection as the dG(0) solution of a heat equation with right-hand side $y_t - \Delta y$, similar to earlier works of [CW10] uncontrolled Navier-Stokes equations, [CC12] for controlled Navier-Stokes and [Chr19] for the uncontrolled Allen-Cahn. In our approach below, we do *not* assume any point-wise space-time bound of the fully-discrete solution of the control-to-state mapping and, most crucially we do *not* construct a discrete approximation of the *spectral estimate*. As a result we arrive at an estimate that is valid under the limited regularity assumptions imposed by our optimal control setting. For the numerical analysis of the discrete adjoint to state mapping, the key difficulty involves the proof of discrete stability and error bounds that depend polynomially upon $1/\epsilon$. Indeed, we note that the spectral estimate is not longer valid if we replace y by its discretization and the direct application of the nonlinear Gronwall Lemma will lead to severe restrictions on the size of $\|y_u - y_d\|_{L_2(0,T;L_2(\Omega))}$ and $\|y(T) - y_\Omega\|_{L_2(\Omega)}$ in terms of ϵ . Such restrictions are not practical in the optimal control setting. Our approach is based on a pseudo duality argument that avoids the construction of a discrete approximation of the spectral estimate and the use of a nonlinear Gronwall Lemma resulting to discrete stability estimates. Then, for the derivation of error estimates for the discrete state to adjoint mapping, we employ a *boot-strap* argument. We note that the error analysis of the state to adjoint mapping may be of independent interest, since it concerns a linear singularly perturbed problem under low regularity assumptions on the given data. Combining these estimates, we are able to proceed in a similar fashion to [CC12] to establish the desired estimates for the difference between local optimal controls and their discrete approximations, as well as estimates for the differences between the corresponding state and adjoint state and their discrete approximations.

6.1 Discretization

Let $\{\mathcal{T}_h\}_{h>0}$ be a family of triangulations of $\bar{\Omega}$. To each \mathcal{T}_h to be a conforming, shape-regular and quasi-uniform subdivision such that $\cup_{\tau \in \mathcal{T}_h} \tau = \bar{\Omega}$. With each element $\tau \in \mathcal{T}_h$ we associate two parameters h_τ and ρ_τ , where h_τ is the diameter of τ while ρ_τ is the diameter of the largest ball contained in τ . Then, we define the meshsize parameter as $h := \max_{\tau \in \mathcal{T}_h} h_\tau$. To each \mathcal{T}_h we associate the finite element space:

$$Y_h := \{y_h \in C(\bar{\Omega}); y_h|_\tau \in \mathbb{P}_1(\tau), \forall \tau \in \mathcal{T}_h\} \subset H_0^1(\Omega),$$

with \mathbb{P}_1 denoting the d -variate space of linear polynomials. We recall the following classical inverse estimates:

$$\|v_h\|_{L_3(\Omega)} \leq C_{\text{inv}} h^{-(d/6)} \|v_h\|_{L_2(\Omega)}, \text{ and } \|v_h\|_{H^1(\Omega)} \leq C_{\text{inv}} h^{-1} \|v_h\|_{L_2(\Omega)}. \quad (6.1)$$

Furthermore, we set

$$U_h = \{u_h \in L_2(0, T; L_2(\Omega)); u_h|_\tau \equiv u_\tau \in \mathbb{R}\}.$$

Let $0 = t_0 < t_1 < \dots < t_N = T$. We consider the quasi-uniform partition of the time interval $[0, T]$ into subintervals $J_n := (t_{n-1}, t_n]$ with $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ each time step. Indeed, we assume that there exists a $C_0 > 0$ such that

$$k = \max_{1 \leq n \leq N} k_n < C_0 k_n \text{ for } n = 1, \dots, N. \quad (6.2)$$

Setting $\sigma = (k, h)$, we consider the following fully discrete spaces:

$$\begin{aligned} Y_\sigma &:= \{y_\sigma \in L_2(0, T; H_0^1(\Omega)); y_\sigma|_{J_n} \in Y_h, n = 1, \dots, N\}, \\ U_\sigma &:= \{u_\sigma \in L_2(0, T; L_2(\Omega)); u_\sigma|_{J_n} \in U_h, n = 1, \dots, N\}. \end{aligned}$$

The functions in Y_σ and U_σ are piecewise constant in time. We are looking for discrete controls in U_σ that can be written in the form:

$$u_\sigma = \sum_{n=1}^N \sum_{\tau \in \mathcal{T}_h} u_{n,\tau} \chi_n \chi_\tau, \quad \text{with } u_{n,\tau} \in \mathbb{R},$$

and χ_n , χ_τ the characteristic functions over (t_{n-1}, t_n) and τ , respectively. We consider the convex subset of U_σ :

$$U_{\sigma,ad} = U_\sigma \cap U_{ad} = \{u_\sigma \in U_\sigma : u_{n,\tau} \in [u_a, u_b]\}.$$

Every element of Y_σ can be written in the form

$$y_\sigma = \sum_{n=1}^N y_{n,h} \chi_n, \quad \text{with } y_{n,h} \in Y_h.$$

We fix $y_\sigma(t_n) = y_{n,h}$ in order y_σ to be continuous from the left. Thus, we have $y_\sigma(T) = y_\sigma(t_N) = y_{N,h}$.

To introduce the discrete control problem, we need to define the fully discrete scheme of the state equation (5.2). For any $u \in L_2(0, T; L_2(\Omega))$, the backward

Euler-finite element method (discontinuous-in time- Galerkin dG(0)) reads: for each $n = 1, \dots, N$ and for all $w_h \in Y_h$,

$$\left(\frac{y_{n,h} - y_{n-1,h}}{k_n}, w_h \right) + (\nabla y_{n,h}, \nabla w_h) + \epsilon^{-2} (F(y_{n,h}), w_h) = (u_n, w_h) \quad (6.3)$$

$$y_{0,h} = y_{0h},$$

where

$$u_n = \frac{1}{k_n} \int_{t_{n-1}}^{t_n} u(t) dt, \quad (6.4)$$

$$y_{0h} \in Y_h \text{ s.t. } \|y_0 - y_{0h}\|_{L_2(\Omega)} \leq Ch \text{ and } \|y_{0h}\|_{H^1(\Omega)} \leq C \quad \forall h > 0.$$

Later in Theorem 6.5 we will prove that for any $u \in L_2(0, T; L_2(\Omega))$, (6.3) has a unique solution $y_\sigma(u) \in Y_\sigma$.

Then, we define the discrete control problem as follows:

$$\begin{cases} \min J_\sigma(u_\sigma) \\ u_\sigma \in U_{\sigma,ad}, \end{cases} \quad (6.5)$$

where

$$J_\sigma(u_\sigma) = \frac{1}{2} \int_0^T \int_\Omega |y_\sigma(u_\sigma) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_\Omega |y_\sigma(T) - y_{\Omega,h}|^2 dx \\ + \frac{\mu}{2} \int_0^T \int_\Omega |u_\sigma|^2 dx dt, \quad (6.6)$$

$$y_{\Omega,h} \in Y_h \text{ s.t. } \|y_\Omega - y_{\Omega,h}\|_{L_2(\Omega)} \leq Ch \text{ and } \|y_{\Omega,h}\|_{H^1(\Omega)} \leq C \quad \forall h > 0. \quad (6.7)$$

We begin with the analysis and error estimation of the discrete state equation. The choice of the dG(0) method is due to the low regularity imposed by the optimal control setting.

6.1.1 Analysis of the discrete state problem

Let $y = y_u = G(u)$ and $y_\sigma = y_\sigma(u) \in Y_\sigma$ be a solution to (6.3). We begin by presenting some discrete stability estimates that are useful for the upcoming analysis.

Definition 6.1. We define the projection operator $P_h : L_2(\Omega) \rightarrow Y_h$ through

$$(P_h y, w_h) = (y, w_h) \quad \forall w_h \in Y_h.$$

Also, we define $P_\sigma : C(0, T; L_2(\Omega)) \rightarrow Y_\sigma$ by

$$(P_\sigma y)_{n,h} = P_h y(t_n),$$

for each $n = 1, \dots, N$.

Lemma 6.2. Let y_σ be a solution to (6.5) corresponding to the control function $u \in L_2(0, T; L_2(\Omega))$, and $y_{0h} := P_h y_0$. Then, there exists a constant $C > 0$ independent of $\sigma = (k, h)$, ϵ and $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$, such that

$$\|y_\sigma\|_{L_2(0,T;L_2(\Omega))} + \|y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ \leq C \left(|\Omega_T|^{\frac{1}{2}} + \|y_0\|_{L_2(\Omega)} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{\text{st},1}^{\text{dG}}, \quad (6.8)$$

and

$$\begin{aligned} & \|y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \|y_\sigma\|_{L_2(0,T;H^1(\Omega))} \\ & + \left(\sum_{n=1}^N \|y_{n,h} - y_{n-1,h}\|_{L_2(\Omega)}^2 \right)^{1/2} \leq \frac{C_{st,1}^{\text{dG}}}{\epsilon}. \end{aligned} \quad (6.9)$$

If in addition, $k \leq \frac{3C_0\epsilon^2}{2}$, with C_0 defined by (6.2), then the following estimate holds

$$\begin{aligned} & \|y_\sigma\|_{L_\infty(0,T;H_0^1(\Omega))} + \frac{1}{\epsilon} \|y_\sigma\|_{L_\infty(0,T;L_4(\Omega))}^2 \\ & \leq C \left(\|\nabla y_{0,h}\|_{L_2(\Omega)} + \frac{1}{\epsilon} \|y_{0,h}\|_{L_4(\Omega)}^2 + \frac{|\Omega|^{1/2}}{\epsilon} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{st,2}^{dG}. \end{aligned} \quad (6.10)$$

Proof. The first two stability estimates can be derived by setting $w_h = y_\sigma$ into (6.3) (see also [Chr19, Section 3]). For the proof of the third, we proceed as it follows. We choose $w_h = (y_{n,h} - y_{n-1,h})/k_n$ in (6.3), to get

$$\begin{aligned} & \left\| \frac{y_{n,h} - y_{n-1,h}}{k_n} \right\|_{L_2(\Omega)}^2 + \frac{1}{k_n} (\nabla y_{n,h}, \nabla (y_{n,h} - y_{n-1,h})) + \frac{1}{\epsilon^2 k_n} (y_{n,h}^3, y_{n,h} - y_{n-1,h}) \\ & = \frac{1}{k_n} (u_n, y_{n,h} - y_{n-1,h}) + \frac{1}{\epsilon^2 k_n} (y_{n,h}, y_{n,h} - y_{n-1,h}). \end{aligned}$$

Young's inequality for $p = 4/3$ and $q = 4$, yields

$$\int_\Omega |y_{n,h}^3| |y_{n-1,h}| \, dx \leq \frac{3}{4} \|y_{n,h}\|_{L_4(\Omega)}^4 + \frac{1}{4} \|y_{n-1,h}\|_{L_4(\Omega)}^4.$$

Hence, using Hölder and Young's inequality and after some standard algebra, we deduce that

$$\begin{aligned} & \frac{3}{4} \left\| \frac{y_{n,h} - y_{n-1,h}}{k_n} \right\|_{L_2(\Omega)}^2 + \frac{1}{2k_n} \|\nabla y_{n,h}\|_{L_2(\Omega)}^2 + \frac{1}{2k_n} \|\nabla (y_{n,h} - y_{n-1,h})\|_{L_2(\Omega)}^2 \\ & + \frac{1}{4\epsilon^2 k_n} \|y_{n,h}\|_{L_4(\Omega)}^4 + \frac{1}{2\epsilon^2 k_n} \|y_{n-1,h}\|_{L_2(\Omega)}^2 \\ & \leq \|u_n\|_{L_2(\Omega)}^2 + \frac{1}{2k_n} \|\nabla y_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{4\epsilon^2 k_n} \|y_{n-1,h}\|_{L_4(\Omega)}^4 \\ & + \frac{1}{2\epsilon^2 k_n} \|y_{n,h}\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2 k_n} \|y_{n,h} - y_{n-1,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

Multiplying by k_n , summing from $n = 1$ up to m , for $m = 1, \dots, N$ and using (6.2), yields

$$\begin{aligned} & \frac{3C_0}{2k} \sum_{n=1}^m \|y_{n,h} - y_{n-1,h}\|_{L_2(\Omega)}^2 + \|\nabla y_{m,h}\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \|y_{m,h}\|_{L_4(\Omega)}^4 \\ & \leq \|\nabla y_{0,h}\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \|y_{0,h}\|_{L_4(\Omega)}^4 + \frac{1}{\epsilon^2} \|y_{m,h}\|_{L_2(\Omega)}^2 \\ & + 2\|u\|_{L_2(0,t_m;L_2(\Omega))}^2 + \frac{1}{\epsilon^2} \sum_{n=1}^m \|y_{n,h} - y_{n-1,h}\|_{L_2(\Omega)}^2. \end{aligned} \quad (6.11)$$

We use Young's inequality to further estimate

$$\frac{1}{\epsilon^2} \|y_{m,h}\|_{L_2(\Omega)}^2 \leq \frac{1}{4\epsilon^2} \|y_{m,h}\|_{L_4(\Omega)}^4 + \frac{|\Omega|}{\epsilon^2}.$$

Finally, selecting k such that, i.e., $\frac{1}{\epsilon^2} \leq \frac{3C_0}{2k}$, in a way to hide the last term on the right-hand side of (6.11) on the left, we deduce the desired estimate. \square

Lemma 6.3. [CC19, Lemma 3.4] There exists a constant $C > 0$ independent of σ such that for every $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ it holds that

$$\begin{aligned}\|y - P_\sigma y\|_{L_2(0,T;L_2(\Omega))} &\leq C \left(k \|y_t\|_{L_2(0,T;L_2(\Omega))} + h^2 \|y\|_{L_2(0,T;H^2(\Omega))} \right), \\ \|y - P_\sigma y\|_{L_2(0,T;H_0^1(\Omega))} &\leq C \left(\sqrt{k} \|y_t\|_{L_2(0,T;L_2(\Omega))} + (\sqrt{k} + h) \|y\|_{L_2(0,T;H^2(\Omega))} \right).\end{aligned}$$

Another technical tool is the definition of a global space-time projection onto Y_σ as a discrete solution to the following auxiliary linear parabolic problem. Let $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ be the solution to (5.2) and $y_{0h} := P_h y_0$. We define $\hat{y}_\sigma \in Y_\sigma$ satisfying: for each $n = 1, \dots, N$ and for every $w_h \in Y_h$,

$$\begin{aligned}\left(\frac{\hat{y}_{n,h} - \hat{y}_{n-1,h}}{k_n}, w_h \right) + (\nabla \hat{y}_{n,h}, \nabla w_h) &= (\hat{f}_n, w_h) \\ \hat{y}_{0,h} &= y_{0h},\end{aligned}\tag{6.12}$$

where,

$$\begin{aligned}(\hat{f}_n, w_h) &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \{(\nabla y(t), \nabla w_h) + (y_t(t), w_h)\} dt \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (\nabla y(t), \nabla w_h) dt + \left(\frac{y(t_n) - y(t_{n-1})}{k_n}, w_h \right).\end{aligned}\tag{6.13}$$

According to [CC14, Lemma 4.6], (6.12) has a unique solution $\hat{y}_\sigma \in Y_\sigma$. We split the error as follows:

$$\hat{e} = y - \hat{y}_\sigma = (y - P_\sigma y) + (P_\sigma y - \hat{y}_\sigma).\tag{6.14}$$

Substituting (6.13) into (6.12), we note that \hat{e} satisfies the following orthogonality condition,

$$\left(\hat{e}(t_n) - \hat{e}(t_{n-1}), w_h \right) + \int_{t_{n-1}}^{t_n} (\nabla \hat{e}, \nabla w_h) dt = 0,\tag{6.15}$$

for all $w_h \in Y_h$ and for each $n = 1, \dots, N$.

The following Lemma collects various stability and error estimates.

Lemma 6.4. Suppose that $\hat{y}_\sigma \in Y_\sigma$ is the solution to (6.12). Then, there exists $C > 0$ independent of σ , such that

$$\|y - \hat{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \|y - \hat{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq C(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)},\tag{6.16}$$

$$\|y - \hat{y}_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq C(k + h^2) \|y\|_{H^{2,1}(\Omega_T)}.\tag{6.17}$$

In addition, there exists a constant $C > 0$ independent of σ, ϵ , such that

$$\|\hat{y}_\sigma\|_{L_\infty(0,T;H_0^1(\Omega))} \leq C \|y\|_{H^{2,1}(\Omega_T)}.\tag{6.18}$$

Proof. In view of Lemma 6.3, (6.16) is immediate. As for the estimation of the second one, that belongs on Y_σ , we refer the readers to the standard techniques presented in [CW06a, CW10], [CC19] and [CC14]. (For completeness we present the proof also in Appendix A). \square

The following result states the main error estimate for the control to state mapping. We emphasise that, unlike previous works for the uncontrolled Allen-Cahn equation, we do not exceed the $H^{2,1}(\Omega_T)$ regularity. Our technique employs the spectral estimate at the “continuous level” and, hence it avoids the construction of discrete approximations, which typically lead to higher regularity requirements. For the purpose of the analysis, we decide to present two different theorems for $d = 2$ and 3, respectively.

Theorem 6.5 (d=2). Let $u \in L_2(0, T; L_2(\Omega))$, $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ and $y_\sigma \in Y_\sigma$ satisfy (5.2) and (6.3) respectively. Suppose that (3.20) holds with $\|\lambda\|_{L_\infty(0,T)} \leq C$, where $C > 0$ a ϵ -independent constant. If there exists $C > 0$ such that

$$\begin{aligned} & (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}^{1/2} \max \left\{ \frac{C_\infty}{\epsilon}, \|y\|_{H^{2,1}(\Omega_T)} \right\}^{1/2} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{1/2} \\ & \leq \epsilon^2 C E^{-1/2}, \end{aligned} \quad (6.19)$$

then, the following estimates hold:

$$\begin{aligned} & \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ & \leq \max \left\{ \frac{C_I}{\epsilon^2} (\sqrt{k} + h), \frac{C_{II}}{\epsilon} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}, C \right\} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}, \end{aligned} \quad (6.20)$$

$$\begin{aligned} & \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \max \left\{ \frac{C_I}{\epsilon^3} (\sqrt{k} + h), \frac{C_{II}}{\epsilon^2} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}, C \right\} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}. \end{aligned} \quad (6.21)$$

Here, we denote by $C_I := 2E^{1/2}C_\infty$, $C_{II} := CE^{1/2}$ and $E := \exp(2T\alpha)$ where

$$C_\infty := C \left(1 + (1 + \epsilon^2) \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 \right)^{1/2}, \quad \alpha := \sup_{t \in [0, T]} (2\lambda(t)(1 - \epsilon^2) + 4),$$

and $C > 0$ an algebraic constant (that might be different in each occurrence) but independent of σ, ϵ , and $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$.

Furthermore, the fully discrete scheme (6.3) admits a unique solution.

Remark 6.6. None of the above constants depend on $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$ exponentially. Indeed, C_I depends on the $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$ polynomially while throughout the analysis $C > 0$ is an algebraic constant independent of $\epsilon, \sigma = (h, k)$ and $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$. We mainly focus on the case where $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$ is bounded independent $1/\epsilon$ (see Remark 6.8 for a detailed discussion). However, our results hold, without any exponential dependence upon $1/\epsilon$ even in more general cases where we no longer assume the aforementioned assumption. In such a case, the condition among σ and ϵ become more restrictive. In particular, we expect to exhibit higher ϵ -dependence.

Proof. We begin by splitting the total error:

$$e = y - y_\sigma = (y - \hat{y}_\sigma) + (\hat{y}_\sigma - y_\sigma) =: \hat{e} + e_\sigma. \quad (6.22)$$

The aim of our analysis is to bound the term e_σ in terms of \hat{e} , whose bounds are known from Lemma 6.4. From (5.5) and (6.3), for all $w_h \in Y_h$, $n = 1, \dots, N$, it holds that

$$(e(t_n) - e(t_{n-1}), w_h) + \int_{t_{n-1}}^{t_n} (\nabla e(t), \nabla w_h) + \epsilon^{-2} (F(y) - F(y_{n,h}), w_h) dt = 0.$$

Using (6.22), the orthogonality condition (6.15) and choosing $w_h = e_{n,h}$, we obtain

$$(e_{n,h} - e_{n-1,h}, e_{n,h}) + \int_{t_{n-1}}^{t_n} \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F(y) - F(y_{n,h}), e_{n,h}) dt = 0.$$

A standard algebraic manipulation implies that

$$F(y) - F(y_{n,h}) = (3y^2 - 1)(y - y_{n,h}) - 3y(y - y_{n,h})^2 + (y - y_{n,h})^3.$$

Using the decomposition (6.22) and elementary identities, we deduce that

$$\begin{aligned} & \frac{1}{2} \|e_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|e_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \\ & + \epsilon^{-2} \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_4(\Omega)}^4 dt + 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} (\hat{e}^2, e_{n,h}^2) dt \\ & + \int_{t_{n-1}}^{t_n} \left(\|\nabla e_{n,h}\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(y)e_{n,h}, e_{n,h}) \right) dt \\ & = -\epsilon^{-2} \int_{t_{n-1}}^{t_n} (F'(y)\hat{e}, e_{n,h}) dt + 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} (y\hat{e}^2, e_{n,h}) dt \\ & + 6\epsilon^{-2} \int_{t_{n-1}}^{t_n} (y\hat{e}, e_{n,h}^2) dt - \epsilon^{-2} \int_{t_{n-1}}^{t_n} (\hat{e}^3, e_{n,h}) dt \\ & - 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} (\hat{e}, e_{n,h}^3) dt + 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} (y, e_{n,h}^3) dt =: \sum_{j=1}^6 \mathcal{I}_j. \end{aligned} \tag{6.23}$$

First, we recover additional coercivity on the right-hand side by employing the spectral estimate at the “continuous level” (3.20) for $v = e_{n,h}$. Indeed, we have

$$\begin{aligned} & \int_{t_{n-1}}^{t_n} \left(\|\nabla e_{n,h}\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(y)e_{n,h}, e_{n,h}) \right) dt \\ & \geq \int_{t_{n-1}}^{t_n} ((\epsilon^2 - 1)\lambda(t) - 1) \|e_{n,h}\|_{L_2(\Omega)}^2 dt + \epsilon^2 \int_{t_{n-1}}^{t_n} \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 dt \\ & + 3 \int_{t_{n-1}}^{t_n} \|ye_{n,h}\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

We estimate the right-hand side of (6.23). Hölder and Young's inequalities yield

$$\begin{aligned}\mathcal{I}_1 &\leq \int_{t_{n-1}}^{t_n} \|ye_{n,h}\|_{L_2(\Omega)}^2 dt + \frac{1}{4\epsilon^4} \int_{t_{n-1}}^{t_n} \left(9\|y\|_{L_\infty(\Omega)}^2 + 1\right) \|\hat{e}\|_{L_2(\Omega)}^2 dt \\ &\quad + \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_2(\Omega)}^2 dt, \\ \mathcal{I}_2 &\leq \frac{1}{2\epsilon^2} \int_{t_{n-1}}^{t_n} \|\hat{e}e_{n,h}\|_{L_2(\Omega)}^2 dt + \frac{9}{2\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)}^2 \|\hat{e}\|_{L_2(\Omega)}^2 dt, \\ \mathcal{I}_3 &\leq \frac{36}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)}^2 \|\hat{e}\|_{L_2(\Omega)}^2 dt + \frac{1}{4\epsilon^2} \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_4(\Omega)}^4 dt, \\ \mathcal{I}_4 &\leq \frac{3}{4\epsilon^2} \int_{t_{n-1}}^{t_n} \|\hat{e}\|_{L_4(\Omega)}^4 dt + \frac{1}{4\epsilon^2} \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_4(\Omega)}^4 dt, \\ \mathcal{I}_5 &\leq \frac{3^7}{4\epsilon^2} \int_{t_{n-1}}^{t_n} \|\hat{e}\|_{L_4(\Omega)}^4 dt + \frac{1}{4\epsilon^2} \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_4(\Omega)}^4 dt.\end{aligned}$$

Similarly, applying Hölder, (2.4), and Young's inequalities we deduce,

$$\begin{aligned}\mathcal{I}_6 &\leq \frac{3\tilde{c}}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_2(\Omega)}^2 \|\nabla e_{n,h}\|_{L_2(\Omega)} dt \\ &\leq \frac{6\tilde{c}}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \|\nabla e_{n,h}\|_{L_2(\Omega)} dt \\ &\quad + \frac{6\tilde{c}}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n-1,h}\|_{L_2(\Omega)}^2 \|\nabla e_{n,h}\|_{L_2(\Omega)} dt \\ &\leq \frac{6\tilde{c}}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \|\nabla e_{n,h}\|_{L_2(\Omega)} dt \\ &\quad + \frac{36\tilde{c}^2}{\epsilon^6} \int_{t_{n-1}}^{t_n} \|e_{n-1,h}\|_{L_2(\Omega)}^4 dt + \frac{\epsilon^2}{4} \int_{t_{n-1}}^{t_n} \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 dt.\end{aligned}$$

We want to ensure that the first term of the bound of \mathcal{I}_6 can be absorbed by the term $\frac{1}{2}\|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2$ on the left-hand side of (6.23). To do so, we can further bound this term as follows:

$$\begin{aligned}&\frac{6\tilde{c}}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \|\nabla e_{n,h}\|_{L_2(\Omega)} dt \\ &\leq 6\tilde{c} \|y\|_{L_\infty(J_n; L_\infty(\Omega))} \frac{k_n}{\epsilon^2} \left(\|y_\sigma\|_{L_\infty(0, T; H_0^1(\Omega))} + \|\hat{y}_\sigma\|_{L_\infty(0, T; H_0^1(\Omega))} \right),\end{aligned}$$

then, through (6.10) and (6.18), we conclude to the following assumption

$$6\tilde{c} \|y\|_{L_\infty(J_n; L_\infty(\Omega))} \frac{k_n}{\epsilon^2} (C_{st,2}^{\text{dG}} + \|y\|_{H^{2,1}(\Omega_T)}) \leq \frac{1}{4}. \quad (6.24)$$

Recalling (3.20) for $v = e_{n,h}$ and inserting the bounds of \mathcal{I}_i into (6.23), we deduce

$$\begin{aligned} & \|e_{n,h}\|_{L_2(\Omega)}^2 - \|e_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \\ & + \frac{1}{2\epsilon^2} \int_{t_{n-1}}^{t_n} \|e_{n,h}\|_{L_4(\Omega)}^4 dt + 2\epsilon^2 \int_{t_{n-1}}^{t_n} \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 dt \\ & + \frac{5}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|\hat{e}e_{n,h}\|_{L_2(\Omega)}^2 dt + 4 \int_{t_{n-1}}^{t_n} \|ye_{n,h}\|_{L_2(\Omega)}^2 dt \\ & \leq \int_{t_{n-1}}^{t_n} \left(\left(\left(\frac{9}{2\epsilon^4} + \frac{81}{\epsilon^2} \right) \|y\|_{L_\infty(\Omega)}^2 + \frac{1}{2\epsilon^4} \right) \|\hat{e}\|_{L_2(\Omega)}^2 + \frac{2 \cdot 3^7}{\epsilon^2} \|\hat{e}\|_{L_4(\Omega)}^4 \right) dt \quad (6.25) \\ & + \int_{t_{n-1}}^{t_n} (2\lambda(t)(1 - \epsilon^2) + 4) \|e_{n,h}\|_{L_2(\Omega)}^2 dt \\ & + \frac{24}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n-1,h}\|_{L_3(\Omega)}^3 dt. \end{aligned}$$

Summing from $n = 1$ up to m , $m = 1, \dots, N$ and dropping positive terms from the left-hand side, we obtain

$$\begin{aligned} & \|e_{m,h}\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \sum_{n=1}^m k_n \|e_{n,h}\|_{L_4(\Omega)}^4 + \frac{3}{2} \epsilon^2 \sum_{n=1}^m k_n \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 \\ & \leq A + \sum_{n=1}^m k_n \alpha \|e_{n,h}\|_{L_2(\Omega)}^2 + \frac{36\tilde{c}^2}{\epsilon^6} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)}^2 \|e_{n,h}\|_{L_2(\Omega)}^4 dt, \quad (6.26) \end{aligned}$$

where $\alpha := \sup_{t \in [0,T]} (2\lambda(t)(1 - \epsilon^2) + 4)$ and

$$\begin{aligned} A := & \left(\left(\frac{9}{2\epsilon^4} + \frac{81}{\epsilon^2} \right) \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 + \frac{1}{2\epsilon^4} \right) \|\hat{e}\|_{L_2(0,T;L_2(\Omega))}^2 \\ & + \frac{2 \cdot 3^7}{\epsilon^2} \|\hat{e}\|_{L_4(0,T;L_4(\Omega))}^4. \end{aligned}$$

Assume that $\sup_{n=1,\dots,N} k_n \alpha \leq 1/2$. Note that for every $m = 1, \dots, N$

$$\begin{aligned} & \frac{36\tilde{c}^2}{\epsilon^6} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)}^2 \|e_{n,h}\|_{L_2(\Omega)}^4 dt \\ & \leq \frac{36\tilde{c}^2}{\epsilon^6} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 \sup_{n=1,\dots,m-1} \|e_{n,h}\|_{L_2(\Omega)}^2 \sum_{n=1}^{m-1} k_n \|e_{n,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

Then, applying Lemma 2.6, we deduce

$$\sup_{n=1,\dots,N} \|e_{n,h}\|_{L_2(\Omega)}^2 + 2\epsilon^2 \sum_{n=1}^N k_n \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 + \frac{2}{\epsilon^2} \sum_{n=1}^N k_n \|e_{n,h}\|_{L_4(\Omega)}^4 \leq 4AE.$$

The above estimate holds, upon setting 2.6 $\beta = 1$ and $B = 36\epsilon^{-6}\tilde{c}^2 \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2$ in Lemma (2.6) as long as

$$\begin{aligned} A & \leq \epsilon^6 \left(16 \cdot 36\tilde{c}^4 \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 (T+1)E^2 \right)^{-1} \quad (6.27) \\ & = \epsilon^6 C_T E^{-2} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{-2}, \end{aligned}$$

with $C_T := 36\tilde{c}^4(T + 1)$, is satisfied. To quantify the dependence of k, h upon ϵ through (6.27) observe that (2.3) and Lemma 6.4, implies

$$\begin{aligned} A &\sim \frac{C_\infty^2}{\epsilon^4} \|y - \hat{y}_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + \frac{C\tilde{c}^4}{\epsilon^2} \|y - \hat{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 \|y - \hat{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))}^2 \\ &\sim \frac{C_\infty^2}{\epsilon^4} (k+h^2)^2 \|y\|_{H^{2,1}(\Omega_T)}^2 + \frac{C\tilde{c}^4}{\epsilon^2} (k+h^2)^2 \|y\|_{H^{2,1}(\Omega_T)}^4, \end{aligned}$$

that along with (6.33) yield the condition:

$$(k+h^2)^2 \|y\|_{H^{2,1}(\Omega_T)}^2 \max \left\{ \frac{C_\infty^2}{\epsilon^2}, C\tilde{c}^4 \|y\|_{H^{2,1}(\Omega_T)}^2 \right\} \leq \epsilon^8 C_T E^{-2} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{-2}.$$

Observe that if the above estimate is satisfied then (6.24) also holds. The estimate follows by triangle inequality and the estimate of Lemma 6.4.

To conclude the proof, we have to show the uniqueness of a solution of (6.3). Let $y_\sigma^1, y_\sigma^2 \in Y_\sigma$ be two solutions to (6.3). We set $\tilde{y}_\sigma = y_\sigma^2 - y_\sigma^1$ and will prove that $\tilde{y}_\sigma = 0$. Subtracting the equations satisfied by y_σ^2 and y_σ^1 and setting $w_{n,h} = \tilde{y}_{n,h}$, we get

$$\begin{aligned} &(\tilde{y}_{n,h} - \tilde{y}_{n-1,h}, \tilde{y}_{n,h}) + k_n \|\nabla \tilde{y}_{n,h}\|_{L_2(\Omega)}^2 + k_n \epsilon^{-2} ((y_{n,h}^2)^3 - (y_{n,h}^1)^3, \tilde{y}_{n,h}) \\ &= k_n \epsilon^{-2} \|\tilde{y}_{n,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

Note that

$$\begin{aligned} &((y_{n,h}^2)^3 - (y_{n,h}^1)^3, \tilde{y}_{n,h}) = ((y_{n,h}^2 - y_{n,h}^1)((y_{n,h}^2)^2 + y_{n,h}^1 y_{n,h}^2 + (y_{n,h}^1)^2), \tilde{y}_{n,h}) \\ &= \|\tilde{y}_{n,h} y_{n,h}^2\|_{L_2(\Omega)}^2 + \|\tilde{y}_{n,h} y_{n,h}^1\|_{L_2(\Omega)}^2 + (\tilde{y}_{n,h} y_{n,h}^1 y_{n,h}^2, \tilde{y}_{n,h}). \end{aligned}$$

Using this in the above identity, we have

$$\begin{aligned} &\frac{1}{2} \|\tilde{y}_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|\tilde{y}_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\tilde{y}_{n,h} - \tilde{y}_{n-1,h}\|_{L_2(\Omega)}^2 + k_n \|\nabla \tilde{y}_{n,h}\|_{L_2(\Omega)}^2 \\ &+ \epsilon^{-2} k_n \|y_{n,h} y_{n,h}^2\|_{L_2(\Omega)}^2 + \epsilon^{-2} k_n \|\tilde{y}_{n,h} y_{n,h}^1\|_{L_2(\Omega)}^2 \\ &= \epsilon^{-2} k_n \|\tilde{y}_{n,h}\|_{L_2(\Omega)}^2 - \epsilon^{-2} k_n (\tilde{y}_{n,h} y_{n,h}^1, y_{n,h}^2 \tilde{y}_{n,h}) \\ &\leq \epsilon^{-2} k_n \|\tilde{y}_{n,h}\|_{L_2(\Omega)}^2 + \frac{\epsilon^{-2} k_n}{2} \|\tilde{y}_{n,h} y_{n,h}^2\|_{L_2(\Omega)}^2 + \frac{\epsilon^{-2} k_n}{2} \|\tilde{y}_{n,h} y_{n,h}^1\|_{L_2(\Omega)}^2, \end{aligned}$$

hence

$$\begin{aligned} &(1 - 2\epsilon^{-2} k_n) \|\tilde{y}_{n,h}\|_{L_2(\Omega)}^2 + \|\tilde{y}_{n,h} - \tilde{y}_{n-1,h}\|_{L_2(\Omega)}^2 + 2k_n \|\nabla \tilde{y}_{n,h}\|_{L_2(\Omega)}^2 \\ &+ \epsilon^{-2} k_n \|\tilde{y}_{n,h} y_{n,h}^2\|_{L_2(\Omega)}^2 + \epsilon^{-2} k_n \|\tilde{y}_{n,h} y_{n,h}^1\|_{L_2(\Omega)}^2 \leq \|\tilde{y}_{n-1,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

If $\epsilon^{-2} k_n \leq 1/4$, for all $n = 1, \dots, N$, which is satisfied due to (6.19), discrete Gronwall inequality and the fact that $\tilde{y}_{0,h} = 0$ imply that $y_\sigma = 0$. \square

Theorem 6.7 (d=3). Let $u \in L_2(0, T; L_2(\Omega))$, $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ and $y_\sigma \in Y_\sigma$ satisfy (5.2) and (6.3) respectively. Suppose that (3.20) holds with $\|\lambda\|_{L_\infty(0,T)} \leq C$, where $C > 0$ a ϵ -independent constant. If there exists $C > 0$ such that

$$(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}^{4/3} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{2/3} \leq \epsilon^3 C E^{-1}, \quad (6.28)$$

then, the following estimates hold:

$$\begin{aligned} & \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ & \leq \max \left\{ \frac{C_{II}}{\epsilon} (\sqrt{k} + h)^{1/2} \|y\|_{H^{2,1}(\Omega_T)}, C \right\} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}, \end{aligned} \quad (6.29)$$

$$\begin{aligned} & \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \max \left\{ \frac{C_{II}}{\epsilon^2} (\sqrt{k} + h)^{1/2} \|y\|_{H^{2,1}(\Omega_T)}, C \right\} (\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}. \end{aligned} \quad (6.30)$$

Here, we denote by $C_I := 2E^{1/2}C_\infty$, $C_{II} := CE^{1/2}$ and $E := \exp(2T\alpha)$ where

$$C_\infty := C \left(1 + (1 + \epsilon^2) \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 \right)^{1/2}, \quad \alpha := \sup_{t \in [0,T]} (2\lambda(t)(1 - \epsilon^2) + 4),$$

and $C > 0$ an algebraic constant (that might be different in each occurrence) but independent of σ , ϵ , and $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$.

Proof. Starting from (6.23), we shall present only the part of the proving steps that are different compared to the $d = 2$ -case. The bounds of \mathcal{I}_i , for $i = 1, \dots, 5$ remain the same while the bound of \mathcal{I}_6 for $d = 3$ differs from one for $d = 2$. Specifically,

$$\begin{aligned} \mathcal{I}_6 & \leq \frac{3}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_3(\Omega)}^3 dt \\ & \leq \frac{12}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h} - e_{n-1,h}\|_{L_3(\Omega)}^3 dt \\ & \quad + \frac{12}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n-1,h}\|_{L_3(\Omega)}^3 dt. \end{aligned}$$

We want to ensure that the first term of the above bound of \mathcal{I}_6 can be absorbed by the term $\frac{1}{2} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2$ on the left-hand side of (6.23). Using (2.4) and (6.1) yields

$$\|e_{n,h} - e_{n-1,h}\|_{L_3(\Omega)}^3 \leq \frac{C_{\text{inv}} \tilde{c}^3}{\sqrt{h}} \|e_{n,h} - e_{n-1,h}\|_{L_2(\Omega)}^2 \|\nabla(e_{n,h} - e_{n-1,h})\|_{L_2(\Omega)}.$$

We can bound the quantity $\|\nabla(e_{n,h} - e_{n-1,h})\|_{L_2(\Omega)}$ by (6.10) and (6.18). Therefore, it is enough to assume that for all $n = 1, \dots, N$ it holds

$$12\tilde{c}^3 C_{\text{inv}} \|y\|_{L_\infty(J_n; L_\infty(\Omega))} \frac{k_n}{\epsilon^2 \sqrt{h}} (C_{\text{st},2}^{\text{dG}} + \|y\|_{H^{2,1}(\Omega_T)}) \leq \frac{1}{4}. \quad (6.31)$$

Recalling (3.20) for $v = e_{n,h}$ and inserting the bounds of \mathcal{I}_i into (6.23), we deduce to (6.25). Acting analogously to the $d = 2$ -case, we sum from $n=1$ up to m , $m = 1, \dots, N$ and drop the positive terms from the left-hand side to obtain

$$\begin{aligned} & \|e_{m,h}\|_{L_2(\Omega)}^2 + \frac{1}{2\epsilon^2} \sum_{n=1}^m k_n \|e_{n,h}\|_{L_4(\Omega)}^4 + 2\epsilon^2 \sum_{n=1}^m k_n \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 \\ & \leq A + \sum_{n=1}^m k_n \alpha \|e_{n,h}\|_{L_2(\Omega)}^2 + \frac{24}{\epsilon^2} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_3(\Omega)}^3 dt, \end{aligned} \quad (6.32)$$

where $\alpha := \sup_{t \in [0, T]} (2\lambda(t)(1 - \epsilon^2) + 4)$ and

$$\begin{aligned} A &:= \left(\left(\frac{9}{2\epsilon^4} + \frac{81}{\epsilon^2} \right) \|y\|_{L_\infty(0, T; L_\infty(\Omega))}^2 + \frac{1}{2\epsilon^4} \right) \|\hat{e}\|_{L_2(0, T; L_2(\Omega))}^2 \\ &\quad + \frac{2 \cdot 3^7}{\epsilon^2} \|\hat{e}\|_{L_4(0, T; L_4(\Omega))}^4. \end{aligned}$$

Assume that $\sup_{n=1, \dots, N} k_n \alpha \leq 1/2$. Note that for every $m = 1, \dots, N$, (2.4) and Young's inequalities (with $p = 4$ and $q = 4/3$) and standard algebra imply that

$$\begin{aligned} &\frac{24}{\epsilon^2} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_3(\Omega)}^3 dt \\ &\leq \frac{24\tilde{c}^3}{\epsilon^2} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_2(\Omega)}^{3/2} \|\nabla e_{n,h}\|_{L_2(\Omega)}^{3/2} dt \\ &= \frac{24\tilde{c}^3}{\epsilon^{7/2}} \sum_{n=1}^{m-1} \int_{t_{n-1}}^{t_n} \|y\|_{L_\infty(\Omega)} \|e_{n,h}\|_{L_2(\Omega)} \left(\|e_{n,h}\|_{L_2(\Omega)}^{1/2} \epsilon^{3/2} \|\nabla e_{n,h}\|_{L_2(\Omega)}^{3/2} \right) dt \\ &\leq \frac{24\tilde{c}^3}{\epsilon^{7/2}} \|y\|_{L_\infty(0, T; L_\infty(\Omega))} \\ &\quad \sup_{n=1, \dots, m-1} \|e_{n,h}\|_{L_2(\Omega)} \sum_{n=1}^{m-1} k_n \left(\|e_{n,h}\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 \right). \end{aligned}$$

Then, applying Lemma 2.6, we deduce

$$\sup_{n=1, \dots, N} \|e_{n,h}\|_{L_2(\Omega)}^2 + 2\epsilon^2 \sum_{n=1}^N k_n \|\nabla e_{n,h}\|_{L_2(\Omega)}^2 + \frac{2}{\epsilon^2} \sum_{n=1}^N k_n \|e_{n,h}\|_{L_4(\Omega)}^4 \leq 4AE.$$

The above estimate holds, upon setting $\beta = 1/2$ and $B = 24\epsilon^{-7/2}\tilde{c}\|y\|_{L_\infty(0, T; L_\infty(\Omega))}$ in Lemma 2.6 as long as

$$\begin{aligned} A &\leq \epsilon^7 \left(192\tilde{c}\|y\|_{L_\infty(0, T; L_\infty(\Omega))}(T+1)E^{3/2} \right)^{-2} \\ &= \epsilon^7 C_T E^{-3} \|y\|_{L_\infty(0, T; L_\infty(\Omega))}^{-2}, \end{aligned} \tag{6.33}$$

where $C_T := 192\tilde{c}(T+1)$. To quantify the relation between k, h and ϵ from (6.33), observe that Lemma 6.4 and the embedding $H^{2,1}(\Omega_T) \subset C(0, T; H^1(\Omega))$ imply $\|y - \hat{y}_\sigma\|_{L_\infty(0, T; H^1(\Omega))} \leq C\|y\|_{H^{2,1}(\Omega_T)}$. Hence, denoting by $C_\infty^2 := C(1 + (1 + \epsilon^2)\|y\|_{L_\infty(0, T; L_\infty(\Omega))}^2)$ where C is an algebraic constant, (2.5) and Lemma 6.4 imply

$$\begin{aligned} A &\sim \frac{C_\infty^2}{\epsilon^4} \|y - \hat{y}_\sigma\|_{L_2(0, T; L_2(\Omega))}^2 \\ &\quad + \frac{C\tilde{c}^4 \|y\|_{H^{2,1}(\Omega)}^2}{\epsilon^2} \|y - \hat{y}_\sigma\|_{L_\infty(0, T; L_2(\Omega))} \|y - \hat{y}_\sigma\|_{L_2(0, T; H_0^1(\Omega))}^2 \\ &\sim \frac{C_\infty^2}{\epsilon^4} (k + h^2)^2 \|y\|_{H^{2,1}(\Omega_T)}^2 + \frac{C\tilde{c}^4}{\epsilon^2} (\sqrt{k} + h)^3 \|y\|_{H^{2,1}(\Omega_T)}^4. \end{aligned}$$

It is clear that if

$$\sqrt{k} + h \leq \frac{\epsilon^2}{C_\infty^2} \|y\|_{H^{2,1}(\Omega_T)}^2 \tag{6.34}$$

then the second term of (6.1.1) dominates the above quantity, and hence (6.1.1) and (6.33) result to the following restriction:

$$(\sqrt{k} + h)^3 \|y\|_{H^{2,1}(\Omega_T)}^4 \tilde{c}^4 C \leq \epsilon^9 C_T E^{-3} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{-2},$$

where $C_T > 0$ is independent of k, h, ϵ , and $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$, $\|y\|_{H^{2,1}(\Omega_T)}$. The estimates (6.29) and (6.30) follow by triangle inequality and the estimate of Lemma 6.4. Note that if (6.28) is satisfied then both conditions (6.31) and (6.34) are satisfied. \square

Remark 6.8. Recall that $C_I \sim \|y\|_{L_\infty(0,T;L_\infty(\Omega))}$ and $\|y\|_{H^{2,1}(\Omega_T)} \sim \epsilon^{-r}$, for $r \in \{1, 2\}$. Assume that there exists a constant $C > 0$ independent of σ, ϵ such that: $\|y\|_{L_\infty(0,T;L_\infty(\Omega))} \leq C$. Then, even for $r = 2$, the conditions (6.24), (6.31) are less restrictive than (6.19), (6.28). Now, we shall indicate the dominant term in the bounds of Theorems 6.5 and 6.7. Indeed, for $d = 2$, (6.19) becomes

$$(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)} \leq C \epsilon^2 \implies \sqrt{k} + h \leq C \epsilon^{2+r}, \quad (6.35)$$

where C is an algebraic constant depending only on the domain, and $\|\lambda\|_{L_\infty(0,T)}$. Hence, replacing (6.35) into the estimates (6.20) and (6.21) we obtain,

$$\begin{aligned} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 &\leq C(\sqrt{k} + h) \epsilon^{-r}, \\ \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} &\leq C(\sqrt{k} + h) \epsilon^{-r}. \end{aligned}$$

For $d = 3$, we deduce that (6.28) becomes

$$(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}^{4/3} \leq C \epsilon^3 \implies \sqrt{k} + h \leq C \epsilon^{3+(4r/3)}, \quad (6.36)$$

and the estimates (6.29) and (6.30) can be written as

$$\begin{aligned} &\|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ &\leq C \max\{\epsilon^{(1/2)-(r/3)}, 1\} (\sqrt{k} + h) \epsilon^{-r} \\ &\leq \begin{cases} C(\sqrt{k} + h) \epsilon^{-1} & \text{when } r = 1, \\ C(\sqrt{k} + h) \epsilon^{-13/6} & \text{when } r = 2, \end{cases} \leq C(\sqrt{k} + h) \epsilon^{-(7r-1)/6}, \end{aligned}$$

and

$$\|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq C(\sqrt{k} + h) \epsilon^{-(8r+3)/6}.$$

Remark 6.9. If additional regularity is present, i.e. if $\|y\|_{W_4^{2,1}(\Omega_T)} \approx \epsilon^{-r}$, then we observe that, using the maximal parabolic regularity results of [LV17], we may bound

$$\|\hat{e}\|_{L_4(0,T;L_4(\Omega))}^4 \sim (\kappa + h^2)^4 \|y\|_{W_4^{2,1}(\Omega_T)}^4 \sim (\kappa + h^2)^4 \epsilon^{-4r}.$$

Therefore, we easily deduce that $A \sim \frac{C_\infty^2}{\epsilon^4} (k+h^2)^2 \|y\|_{H^{2,1}(\Omega_T)}^2$ for both $d = 2, 3$. As a consequence the conditionality reads as

$$\begin{aligned} \sqrt{k} + h &\sim \epsilon^{2+(r/2)} && \text{when } d = 2, \\ \sqrt{k} + h &\sim \epsilon^{(11/4)+(r/2)} && \text{when } d = 3. \end{aligned}$$

Note that Theorems 6.5, 6.7 and Remark 6.8 play a crucial role in the derivation of the following result.

Corollary 6.10. Let $u, v \in L_2(0, T; L_2(\Omega))$, $y_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ be the solution of (5.2) while $y_\sigma(v) \in Y_\sigma$ the solution of (6.3) corresponding to the control v . Suppose that the assumptions of Theorems 5.5, 6.5 and 6.7 hold. In addition, let $\|y_v\|_{L_\infty(0,T;L_\infty(\Omega))} \leq C$, and $\|y_v\|_{H^{2,1}(\Omega_T)} \leq C\epsilon^{-r}$ with $r \in \{1, 2\}$, where C denotes a constant that depends only on data and it is independent of ϵ and that (6.35) or (6.36) hold for $d = 2$ or 3 , respectively. Then, for $d = 2$

$$\|y_u - y_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} \leq L_1 \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^r} (\sqrt{k} + h), \quad (6.37)$$

$$\|y_u - y_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{L_1}{\epsilon} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^r} (\sqrt{k} + h), \quad (6.38)$$

while for $d = 3$, we have

$$\|y_u - y_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} \leq L_1 \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^{(7r-1)/6}} (\sqrt{k} + h), \quad (6.39)$$

$$\|y_u - y_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{L_1}{\epsilon} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^{(8r+3)/6}} (\sqrt{k} + h). \quad (6.40)$$

Let $u_\sigma \in U_\sigma$. If $u_\sigma \rightharpoonup u$ weakly in $L_2(0, T; L_2(\Omega))$ for every σ ; then

$$\begin{aligned} &\|y_u - y_\sigma(u_\sigma)\|_{L_2(0,T;H_0^1(\Omega))} \rightarrow 0, \\ &\|y_u - y_\sigma(u_\sigma)\|_{L_p(0,T;L_2(\Omega))} \rightarrow 0 \quad \forall 1 \leq p < \infty, \\ &\|y_u(T) - y_\sigma(u_\sigma)(T)\|_{L_2(\Omega)} \rightarrow 0. \end{aligned} \quad (6.41)$$

Proof. Inequalities (6.37), (6.38), (6.39), (6.40) follow from (5.9) and Remark 6.8 using triangle inequality. For (6.41) we split,

$$y_u - y_\sigma(u_\sigma) = (y_u - y_{u_\sigma}) + (y_{u_\sigma} - y_\sigma(u_\sigma)).$$

According to Lemma 5.1 and the boundedness of $\{u_\sigma\}_\sigma$ in $L_2(0, T; L_2(\Omega))$, we have that $\|y_{u_\sigma}\|_{H^{2,1}(\Omega_T)} \leq C_{st}\epsilon^{-r}$, $r \in \{1, 2\}$. Then, any weakly convergent subsequence of $\{y_{u_\sigma}\}_\sigma$ in $H^{2,1}(\Omega_T)$, converges to y_u . Note that the compact embeddings $H^{2,1}(\Omega_T) \subset L_2(0, T; H^1(\Omega))$, $H^{2,1}(\Omega_T) \subset L_p(0, T; L_2(\Omega))$ for $1 \leq p < \infty$ and $H^{2,1}(\Omega_T) \hookrightarrow L_2(\partial\Omega_T)$ imply that

$$\|y_u - y_{u_\sigma}\|_{L_2(0,T;H_0^1(\Omega))} + \|y_u - y_{u_\sigma}\|_{L_p(0,T;L_2(\Omega))} + \|y_u(T) - y_{u_\sigma}(T)\|_{L_2(\Omega)} \rightarrow 0.$$

For every fixed ϵ as $\sigma \rightarrow 0$, with κ, h satisfying the assumptions of Theorems 6.5 and 6.7 for $d = 2$ and $d = 3$, respectively, we deduce

$$\begin{aligned} &\|y_{u_\sigma}(T) - y_\sigma(u_\sigma)(T)\|_{L_2(\Omega)} + \|y_{u_\sigma} - y_\sigma(u_\sigma)\|_{L_2(0,T;H_0^1(\Omega))} \rightarrow 0, \\ &\|y_{u_\sigma} - y_\sigma(u_\sigma)\|_{L_\infty(0,T;L_2(\Omega))} \rightarrow 0, \end{aligned}$$

which completes the proof. \square

The next theorem studies the differentiability of the relation between control and discrete state. The proof follows well known techniques see for instance [CC12, Theorem 4.10].

Theorem 6.11. Let $u, v \in L_2(0, T; L_2(\Omega))$. The mapping

$$G_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow Y_\sigma,$$

such that $y_\sigma = y_\sigma(u) = G_\sigma(u)$, is of class C^∞ . We denote by $z_\sigma(v) = G'_\sigma(u)v$ the unique solution to the problem: For $n = 1, \dots, N$ and for all $w_h \in Y_h$,

$$\begin{aligned} & \left(\frac{z_{n,h} - z_{n-1,h}}{k_n}, w_h \right) + (\nabla z_{n,h}, \nabla w_h) + \epsilon^{-2} ((3y_{n,h}^2 - 1)z_{n,h}, w_h) \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (v(t), w_h) dt, \quad \text{with } z_{0,h} = 0. \end{aligned} \tag{6.42}$$

Proof. We consider the mapping $F_\sigma : Y_\sigma \times L_2(0, T; L_2(\Omega)) \rightarrow Y'_\sigma$ that is defined through $F_\sigma(y_\sigma, u) = g_\sigma$, where

$$\begin{aligned} \langle g_\sigma, w_\sigma \rangle &= \sum_{n=1}^N \left\{ (y_{n,h} - y_{n-1,h}, w_{n,h}) + k_n (\nabla y_{n,h}, \nabla w_{n,h}) \right. \\ &\quad \left. + \epsilon^{-2} k_n (y_{n,h}^3 - y_{n,h}, w_{n,h}) \right\} - \sum_{n=1}^N \int_{t_{n-1}}^{t_n} (u(t), w_h) dt, \end{aligned}$$

for all $w_\sigma \in Y_\sigma$. Note that F_σ is of class C^∞ and $\frac{\partial F_\sigma}{\partial y_\sigma}(y_\sigma, u)z_\sigma = \tilde{g}_\sigma$ is defined through

$$\begin{aligned} \langle \tilde{g}_\sigma, w_\sigma \rangle &= \sum_{n=1}^N \left\{ (z_{n,h} - z_{n-1,h}, w_{n,h}) + k_n (\nabla z_{n,h}, \nabla w_{n,h}) \right\} \\ &\quad + \sum_{n=1}^N \epsilon^{-2} k_n ((3y_{n,h}^2 - 1)z_{n,h}, w_{n,h}), \quad \text{with } z_{0,h} = 0. \end{aligned}$$

We need to ensure that $\frac{\partial F_\sigma}{\partial y_\sigma}(y_\sigma, u)$ is an isomorphism from Y_σ to Y'_σ for all $u \in L_2(0, T; L_2(\Omega))$. Indeed, it suffices to show that is injective because it is a linear mapping between finite dimensional spaces. To do so, assuming that $\frac{\partial F_\sigma}{\partial y_\sigma}(y_\sigma, u)z_\sigma = 0$ for some $z_\sigma \in Y_\sigma$ we will prove that $z_\sigma = 0$. Applying $\frac{\partial F_\sigma}{\partial y_\sigma}(y_\sigma, u)z_\sigma \in Y'_\sigma$ to z_σ , we obtain

$$\begin{aligned} & \frac{1}{2} \|z_{N,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \sum_{n=1}^N \|z_{n,h} - z_{n-1,h}\|_{L_2(\Omega)}^2 + \sum_{n=1}^N k_n \|z_{n,h}\|_{L_2(\Omega)}^2 \\ &+ 3\epsilon^{-2} \sum_{n=1}^N k_n \|y_{n,h} z_{n,h}\|_{L_2(\Omega)}^2 = \frac{1}{2} \|z_{0,h}\|_{L_2(\Omega)}^2 + \epsilon^{-2} \sum_{n=1}^N k_n \|z_{n,h}\|_{L_2(\Omega)}^2 \end{aligned}$$

Discrete Gronwall inequality and the fact that $z_{0,h} = 0$ imply that $z_\sigma = 0$. Furthermore, we have that $F_\sigma(y_\sigma(u), u) = 0$. The Implicit Function Theorem implies that G_σ is of class C^∞ and, thus, we can write $F_\sigma(y_\sigma(u), u) = F_\sigma(y_\sigma(u), u) = 0$ for all $u \in L_2(0, T; L_2(\Omega))$. Then, the chain rule implies that

$$\frac{\partial F_\sigma}{\partial y_\sigma}(y_\sigma(u), u)G'_\sigma(u)v + \frac{\partial F_\sigma}{\partial u}(y_\sigma(u), u)v = 0,$$

for all $v \in L_2(0, T; L_2(\Omega))$. Upon setting $z_\sigma(v) = G'_\sigma(u)v$, (6.42) follows. \square

The key challenge is to prove bounds with constants that do not depend exponentially upon $1/\epsilon$. We observe the absence of the cubic semilinear term and that a discrete analogue of (3.20) cannot be used for $y_{n,h}$. We have already explained that our analysis applies the *spectral estimate* only at the ‘continuous level’, without exceeding the regularity of the state solution that is affordable in the optimal control setting. Hence, the recovery of stability bounds that are independent of the exponential of $1/\epsilon$ is not straightforward. Even if we manage to avoid the exponential dependence on $1/\epsilon$, we seek to derive instead discrete stability bounds that exhibit low polynomial dependence on $1/\epsilon$ at least the same order of the analogous continuous results. A key part of the remaining of our work is to circumvent these difficulties. Our approach is demonstrated later for the discrete adjoint-state equation, but can be applied to (6.42) in a straightforward manner.

6.1.2 Analysis of the discrete adjoint state equation

The differentiability properties of $G_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow Y_\sigma$ imply that the reduced cost functional $J_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow \mathbb{R}$ is of class C^∞ , as well. Applying the chain rule, we get

$$\begin{aligned} J'_\sigma(u)v &= \int_0^T \int_\Omega (y_\sigma - y_d)z_\sigma \, dx \, dt + \gamma \int_\Omega (y_\sigma(T) - y_{\Omega,h})z_\sigma(T) \, dx \\ &\quad + \mu \int_0^T \int_\Omega uv \, dx \, dt, \end{aligned} \tag{6.43}$$

We aim to eliminate z_σ from (6.43). We consider the corresponding fully discrete scheme of the adjoint state equation (5.16), reading: for each $n = N, \dots, 1$ and for all $w_h \in Y_h$, we seek $\varphi_{n,h} = \varphi_\sigma(t_{n-1})$,

$$\begin{aligned} &\left(\frac{\varphi_{n,h} - \varphi_{n+1,h}}{k_n}, w_h \right) + (\nabla \varphi_{n,h}, \nabla w_h) + \epsilon^{-2} ((3y_{n,h}^2 - 1)\varphi_{n,h}, w_h) \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (y_{n,h} - y_d(t), w_h) \, dt, \\ &\varphi_{N+1,h} = \gamma (y_{N,h} - y_{\Omega,h}). \end{aligned} \tag{6.44}$$

The above (backwards in time) fully-discrete equation is understood as follows: we begin by computing $\varphi_{N,h}$ using $\varphi_{N+1,h}$ and then we descend from $n = N$ until $n = 1$. Following the steps from [CC12, Section 4.2], we deduce, respectively,

$$\begin{aligned} &\int_0^T \int_\Omega (y_\sigma - y_d)z_\sigma \, dx \, dt = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} (y_{n,h} - y_d, z_{n,h}) \, dt \\ &= \sum_{n=1}^N \left\{ (\varphi_{n,h} - \varphi_{n+1,h}, z_{n,h}) + k_n (\nabla \varphi_{n,h}, \nabla z_{n,h}) + \epsilon^{-2} k_n ((3y_{n,h}^2 - 1)\varphi_{n,h}, z_{n,h}) \right\} \\ &= - \sum_{n=1}^N (\varphi_{n+1,h}, z_{n,h}) + \sum_{n=1}^N (\varphi_{n,h}, z_{n-1,h}) + \sum_{n=1}^N \int_{t_{n-1}}^{t_n} (v(t), \varphi_{n,h}) \, dt \\ &= - (\varphi_{N+1,h}, z_{N,h}) + (\varphi_{1,h}, z_{0,h}) + \int_0^T \int_\Omega v \varphi_\sigma \, dx \, dt \\ &= - \gamma \int_\Omega (y_\sigma(T) - y_{\Omega,h}) z_\sigma(T) \, dx + \int_0^T \int_\Omega v \varphi_\sigma \, dx \, dt, \end{aligned}$$

since $z_{0,h} = 0$. Thus, the expression (6.43) can be written as

$$J'_\sigma(u)v = \int_0^T \int_\Omega (\varphi_\sigma + \mu u) v \, dx \, dt \quad \forall v \in L_2(0, T; L_2(\Omega)). \quad (6.45)$$

The following projection operator R_σ is the analogue of projection operator P_σ suitably modified to handle the backwards in time problem. Let $R_\sigma : C(0, T; L_2(\Omega)) \rightarrow Y_\sigma$ defined through $(R_\sigma w)_{n,h} = (R_\sigma w)(t_{n-1}) = P_h w(t_{n-1})$, $n = N, \dots, 1$. If $w \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ there exists $C > 0$ such that

$$\|w - R_\sigma w\|_{L_2(0, T; L_2(\Omega))} \leq C \left(k \|w_t\|_{L_2(0, T; L_2(\Omega))} + h^2 \|w\|_{L_2(0, T; H^2(\Omega))} \right), \quad (6.46)$$

$$\|w - R_\sigma w\|_{L_2(0, T; H_0^1(\Omega))} \leq C \left(\sqrt{k} \|w_t\|_{L_2(0, T; L_2(\Omega))} + h \|w\|_{L_2(0, T; H^2(\Omega))} \right), \quad (6.47)$$

$$\|w - R_\sigma w\|_{L_\infty(0, T; L_2(\Omega))} \leq C \left(\sqrt{k} \|w_t\|_{L_2(0, T; L_2(\Omega))} + h \|w\|_{L_\infty(0, T; H^1(\Omega))} \right); \quad (6.48)$$

these follow from standard best approximation results for the L_2 -orthogonal projection.

The following lemma provides the basic stability estimates for the discrete adjoint state problem (6.44). We stress that our approach avoids assumptions regarding the construction of a discrete approximation of the spectral estimate based on a carefully constructed pseudo-duality and boot-strap argument. Indeed, we notice that the lack of a discrete spectral estimate leads to bounds with exponentially dependence on $1/\epsilon$ when combined with standard techniques. To overcome this difficulty we add and subtract the quantity $\epsilon^{-2}(3y^2\varphi_{n,h}, w_h)$ from (6.44). This allows to apply the spectral estimate at the ‘continuous level’ and to use the main error estimates for the control to state mapping $y - y_\sigma$ from Theorems 6.5 and 6.7. Then, through standard argumentation and application of a discrete linear Gronwall Lemma, we obtain conditional type stability estimates using a pseudo-duality approach.

Lemma 6.12. Let $u \in L_2(0, T; L_2(\Omega))$, $y_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ be the solution of (5.2) while $y_\sigma(u) \equiv y_\sigma \in Y_\sigma$ is the solution of (6.3) corresponding to the control u . Suppose that the assumptions of Theorem 5.5 hold. Let also that $C_\infty \sim \|y_u\|_{L_\infty(0, T; L_\infty(\Omega))}$, and $\|y_u\|_{H^{2,1}(\Omega_T)} \leq C\epsilon^{-r}$ with $r \in \{1, 2\}$, where $C > 0$ denotes a constant that depends only on data and it is independent of ϵ and $C_\zeta := \exp \left(\int_0^T 2\lambda(t)(1 - \epsilon^2) + 3 \, dt \right)$, and that (6.35) or (6.36) hold for $d = 2$ or 3, respectively. If, in addition,

$$\begin{aligned} \sqrt{k} + h &\leq \frac{C\epsilon^{2+r}}{C_\infty C_\zeta} && \text{for } d = 2, \\ \sqrt{k} + h &\leq \frac{C\epsilon^{3+(4r/3)}}{C_\infty C_\zeta} && \text{for } d = 3, \end{aligned} \quad (6.49)$$

there exists $D_{st,1}^{\text{dG}} > 0$, independent of $\sigma = (k, h)$ and ϵ , such that:

$$\|\nabla \varphi_\sigma\|_{L_2(0, T; L_2(\Omega))} + \frac{1}{\epsilon} \|y_\sigma \varphi_\sigma\|_{L_2(0, T; L_2(\Omega))} \leq \frac{D_{st,1}^{\text{dG}}}{\epsilon};$$

here, $D_{st,1}^{\text{dG}} := C (\gamma \|y_{N,h} - y_{\Omega,h}\|_{L_2(\Omega)} + \|y_\sigma - y_d\|_{L_2(0, T; L_2(\Omega))})$ with C denoting an algebraic constant independent of ϵ .

Proof. Standard arguments imply the existence and uniqueness of solution φ_σ of (6.44). As usual, we need to develop stability bounds with constants independent of $1/\epsilon$. For this purpose, we employ a duality argument. Given right-hand side φ_σ , we define $\zeta_\sigma \in Y_\sigma$ such that for $n = 1, \dots, N$, and for $w_h \in Y_\sigma$,

$$\begin{aligned} & (\zeta_{n,h} - \zeta_{n-1,h}, w_h) + \int_{t_{n-1}}^{t_n} ((\nabla \zeta_{n,h}, \nabla w_h) + \epsilon^{-2} ((3y^2 - 1)\zeta_{n,h}, w_h)) dt \\ &= \int_{t_{n-1}}^{t_n} (\varphi_{n,h}, w_h) dt, \quad \text{with } \zeta_{0,h} = 0. \end{aligned} \quad (6.50)$$

Setting $w_h = \zeta_{n,h}$ and using the spectral estimate (3.20) at ‘continuous level’ for $v = \zeta_{n,h}$, we easily deduce that

$$\begin{aligned} & \|\zeta_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\nabla \zeta_\sigma\|_{L_2(0,T;L_2(\Omega))} + \|y \zeta_\sigma\|_{L_2(0,T;L_2(\Omega))} \\ & \leq C_\zeta \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}, \end{aligned} \quad (6.51)$$

where $C_\zeta := C \exp \left(\int_0^T 2\lambda(t)(1 - \epsilon^2) + 3 dt \right)$, with C an algebraic constant depending on the domain. Setting now $w_h = (\zeta_{n,h} - \zeta_{n-1,h})/k_n$ into (6.50), and using Hölder and Young’s inequalities, we obtain:

$$\begin{aligned} & \frac{1}{k_n} \left\| \zeta_{n,h} - \zeta_{n-1,h} \right\|_{L_2(\Omega)}^2 + \|\nabla z_{n,h}\|_{L_2(\Omega)}^2 - \|\nabla z_{n-1,h}\|_{L_2(\Omega)}^2 + \|\nabla(\zeta_{n,h} - \zeta_{n-1,h})\|_{L_2(\Omega)}^2 \\ & \leq \left(\frac{3\|y\|_{L_\infty(\Omega)}^2 + 1}{\epsilon^2} \|\zeta_{n,h}\|_{L_2(\Omega)} + \|\varphi_{n,h}\|_{L_2(\Omega)} \right) \left\| \zeta_{n,h} - \zeta_{n-1,h} \right\|_{L_2(\Omega)} \\ & \leq \frac{1}{2k_n} \left\| \zeta_{n,h} - \zeta_{n-1,h} \right\|_{L_2(\Omega)}^2 + \frac{(3\|y\|_{L_\infty(\Omega)}^2 + 1)^2}{\epsilon^4} k_n \|\zeta_{n,h}\|_{L_2(\Omega)}^2 + k_n \|\varphi_{n,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

Summing the above inequalities and using (6.51) we derive the estimate,

$$\|\nabla \zeta_\sigma\|_{L_\infty(0,T;L_2(\Omega))} \leq C_\zeta \left(\frac{C_\infty^2 + 1}{\epsilon^2} + 1 \right) \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}, \quad (6.52)$$

upon setting $C_\infty^2 := 3\|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2$ for brevity. Now we proceed with the duality argument. Setting $w_h = \zeta_{n,h}$ into (6.44) we obtain that

$$\begin{aligned} & (\varphi_{n,h} - \varphi_{n+1,h}, \zeta_{n,h}) + \int_{t_{n-1}}^{t_n} ((\nabla \varphi_{n,h}, \nabla \zeta_{n,h}) + \epsilon^{-2} ((3y_{n,h}^2 - 1)\varphi_{n,h}, \zeta_{n,h})) dt \\ &= \int_{t_{n-1}}^{t_n} (y_{n,h} - y_d(t), \zeta_{n,h}) dt. \end{aligned}$$

Similarly setting $w_h = \varphi_{n,h}$ into (6.50), we have

$$\begin{aligned} & (\zeta_{n,h} - \zeta_{n-1,h}, \varphi_{n,h}) + \int_{t_{n-1}}^{t_n} ((\nabla \varphi_{n,h}, \nabla \zeta_{n,h}) + \epsilon^{-2} ((3y^2 - 1)\zeta_{n,h}, \varphi_{n,h})) dt \\ &= \int_{t_{n-1}}^{t_n} \|\varphi_{n,h}\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

Subtracting the last two equalities and summing them from 1 up to N , we deduce

$$\begin{aligned} & \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ &= (\zeta_{N,h}, \varphi_{N+1,h}) + \int_0^T (y_\sigma - y_d, \zeta_\sigma) dt + \frac{3}{\epsilon^2} \int_0^T ((y^2 - y_\sigma^2)\varphi_\sigma, \zeta_\sigma) dt, \end{aligned} \quad (6.53)$$

where we have used $\zeta_{0,h} = 0$ and the telescopic sum

$$\sum_{n=1}^N \left\{ (\zeta_{n,h} - \zeta_{n-1,h}, \varphi_{n,h}) - (\varphi_{n,h} - \varphi_{n+1,h}, \zeta_{n,h}) \right\} = (\zeta_{N,h}, \varphi_{N+1,h}).$$

Therefore, we may bound the terms of the right-hand side of (6.53), as follows: using the estimates of (6.51) and Young's inequality, we have

$$\begin{aligned} & \int_0^T (y_\sigma - y_d, \zeta_\sigma) dt + (\zeta_{N,h}, \varphi_{N+1,h}) \\ & \leq \|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))} \|\zeta_\sigma\|_{L_2(0,T;L_2(\Omega))} + \|\zeta_{N,h}\|_{L_2(\Omega)} \|\varphi_{N+1,h}\|_{L_2(\Omega)} \\ & \leq \frac{1}{4} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + C_\zeta^2 \left(\|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))}^2 + \|\varphi_{N+1,h}\|_{L_2(\Omega)}^2 \right). \end{aligned} \quad (6.54)$$

For the third term of (6.53), the identity $y^2 - y_\sigma^2 = 2y(y - y_\sigma) - (y - y_\sigma)^2$ yields,

$$\begin{aligned} & \frac{3}{\epsilon^2} \int_0^T ((y^2 - y_\sigma^2)\varphi_\sigma, \zeta_\sigma) dt \\ &= \frac{6}{\epsilon^2} \int_0^T (y(y - y_\sigma)\varphi_\sigma, \zeta_\sigma) dt - \frac{3}{\epsilon^2} \int_0^T (-(y - y_\sigma)^2\varphi_\sigma, \zeta_\sigma) dt. \end{aligned} \quad (6.55)$$

Once again, we need to distinguish the cases $d = 2$ and $d = 3$. For $d = 3$ we work as follows: using Hölder, Poincaré and Young's inequalities (with an appropriate $\delta_1 > 0$ to be chosen later), estimate (6.51) and Theorem 6.5 - Remark 6.8, we may bound the first term of (6.55) as

$$\begin{aligned} & \frac{6}{\epsilon^2} \int_0^T ((y - y_\sigma)y\varphi_\sigma, \zeta_\sigma) dt \\ & \leq \frac{6}{\epsilon^2} \int_0^T \|y - y_\sigma\|_{L_6(\Omega)} \|y\|_{L_\infty(\Omega)} \|\varphi_\sigma\|_{L_3(\Omega)} \|\zeta_\sigma\|_{L_2(\Omega)} dt \\ & \leq \frac{3\tilde{c}^2 C_\infty^2}{2\epsilon^5 \delta_1} \|\zeta_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))}^2 + \epsilon \delta_1 \|\varphi_\sigma\|_{L_2(0,T;L_3(\Omega))}^2 \\ & \leq \frac{3C_\infty^2 C_\zeta^2}{2\delta_1 \epsilon^5} \frac{(k+h^2)}{\epsilon^{(8r/3)+1}} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + \frac{1}{8} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \quad + 2\tilde{c}^2 \epsilon^2 \delta_1^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned}$$

Choosing k, h such that

$$\frac{3C_\infty^2 C_\zeta^2 (k+h^2)}{2\delta_1 \epsilon^{6+(8r/3)}} \leq \frac{1}{8}, \quad (6.56)$$

we obtain

$$\begin{aligned} & \frac{6}{\epsilon^2} \int_0^T ((y - y_\sigma)y\varphi_\sigma, \zeta_\sigma) dt \\ & \leq \frac{1}{4} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + 2\tilde{c}^2 \epsilon^2 \delta_1^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned} \quad (6.57)$$

For the second term on the right-hand side of (6.55), we proceed as follows: for a suitably chosen $\delta_2 > 0$ (to be determined later) we use Hölder and Young's inequalities, the Gagliardo-Nirenberg inequality (2.4), estimates (6.51), (6.52) and the estimates of Theorem 6.5 - Remark 6.8 for $y - y_\sigma$, to get

$$\begin{aligned} & \frac{3}{\epsilon^2} \int_0^T ((y - y_\sigma)^2 \varphi_\sigma, \zeta_\sigma) dt \\ & \leq \frac{3}{\epsilon^2} \int_0^T \|y - y_\sigma\|_{L_4(\Omega)}^2 \|\varphi_\sigma\|_{L_6(\Omega)} \|\zeta_\sigma\|_{L_3(\Omega)} dt \\ & \leq \frac{9\tilde{c}^2}{\delta_2 \epsilon^6} \|\nabla \zeta_\sigma\|_{L_\infty(0,T;L_2(\Omega))} \|\zeta_\sigma\|_{L_\infty(0,T;L_2(\Omega))} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^4 \\ & \quad + \delta_2 \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \leq \frac{9\tilde{c}^2}{\delta_2 \epsilon^6} C_\zeta^2 \left(\frac{C_\infty^2 + 1}{\epsilon^2} + 1 \right) \epsilon^2 \frac{(k + h^2)}{\epsilon^{(7r-1)/3}} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + \delta_2 \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned}$$

Choosing κ, h such that

$$\left(\frac{9}{\delta_2} \right) \frac{\tilde{c}^2}{\epsilon^4} C_\zeta^2 \left(\frac{C_\infty^2 + 1}{\epsilon^2} + 1 \right) \frac{(k + h^2)}{\epsilon^{(7r-1)/3}} \leq \frac{1}{4}, \quad (6.58)$$

there holds that

$$\begin{aligned} & \frac{3}{\epsilon^2} \int_0^T |((y - y_\sigma)^2 \varphi_\sigma, \zeta_\sigma)| dt \\ & \leq \frac{1}{4} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + \delta_2 \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned} \quad (6.59)$$

Substituting (6.57), (6.59) into (6.55) we get

$$\begin{aligned} & \frac{3}{\epsilon^2} \int_0^T ((y^2 - y_\sigma^2) \varphi_\sigma, \zeta_\sigma) dt \\ & \leq \frac{1}{2} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + (2\tilde{c}^2 \delta_1^2 + \delta_2) \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned} \quad (6.60)$$

Thus, returning back to (6.53), upon substituting (6.54) and (6.60), yields

$$\begin{aligned} & \frac{1}{4} \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \leq (2\tilde{c}^2 \delta_1^2 + \delta_2) \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \quad + C_\zeta^2 \left(\|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))}^2 + \|\varphi_{N+1,h}\|_{L_2(\Omega)}^2 \right). \end{aligned} \quad (6.61)$$

Next we employ a boot-strap argument. First, we return to (6.44) and set $w_h = \varphi_{n,h}$ to deduce, after standard algebra,

$$\begin{aligned} & \frac{1}{2} \|\varphi_{0,h}\|_{L_2(\Omega)}^2 + \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + 3\epsilon^{-2} \|y_\sigma \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \leq \left(\frac{1}{2} + \epsilon^{-2} \right) \|\varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + \frac{1}{2} \|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))}^2 + \frac{1}{2} \|\varphi_{N+1,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

We apply (6.61) to substitute the first term of the right-hand side, giving

$$\begin{aligned} & \|\varphi_{0,h}\|_{L_2(\Omega)}^2 + 2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 + 6\epsilon^{-2} \|y_\sigma \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \leq 4 (1 + 2\epsilon^{-2}) (2\tilde{c}^2 \delta_1^2 + \delta_2) \epsilon^2 \|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \\ & \quad + ((1 + 2\epsilon^{-2}) 4C_\zeta^2 + 1) \left(\|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))}^2 + \|\varphi_{N+1,h}\|_{L_2(\Omega)}^2 \right), \end{aligned}$$

Choosing $\delta_1, \delta_2 > 0$ such that $(1 + \frac{2}{\epsilon^2}) 4(2\tilde{c}^2\delta_1^2 + \delta_2)\epsilon^2 \leq 1$, we finally deduce the desired estimate. For $d = 2$, we work completely analogously, using the respective GNL inequality. \square

Theorem 6.13. Let $u \in L_2(0, T; L_2(\Omega))$ and $y, \varphi \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ be the associated state solution of (5.2) and the adjoint state solution of (5.16), respectively. Let y_σ be the associated discrete state solution of (6.3), while φ_σ the associated discrete adjoint state solution of (6.44). Then, under the assumptions of Theorems 6.5, 6.7 and Lemma 6.12 there exists $\hat{C} > 0$ such that, for $r \in \{1, 2\}$, the following estimates hold

$$\|\varphi - \varphi_\sigma\|_{L_\infty(0, T; L_2(\Omega))} + \epsilon \|\varphi - \varphi_\sigma\|_{L_2(0, T; H_0^1(\Omega))} \leq \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{5+r}} \quad \text{for } d = 2, \quad (6.62)$$

$$\|\varphi - \varphi_\sigma\|_{L_\infty(0, T; L_2(\Omega))} + \epsilon \|\varphi - \varphi_\sigma\|_{L_2(0, T; H_0^1(\Omega))} \leq \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{5+(7r-1)/6}} \quad \text{for } d = 3; \quad (6.63)$$

here, we denote by $E := \exp(T\alpha)$ where $\alpha := \sup_{t \in [0, T]} (2\lambda(t)(1 - \epsilon^2) + 5)$ and $\hat{C} := CE^{1/2}D_{st,1}^{\text{dG}}$, where $C > 0$ depending only on the data.

Proof. We split the total error as follows:

$$e := \varphi - \varphi_\sigma = (\varphi - R_\sigma \varphi) + (R_\sigma \varphi - \varphi_\sigma) = \eta + \xi_\sigma. \quad (6.64)$$

For each $n=0, \dots, N-1$ we have,

$$\begin{aligned} \eta(t_n) &= \varphi(t_n) - (R_\sigma \varphi)(t_n) = \varphi(t_n) - (R_\sigma \varphi)_{n+1,h} = \varphi(t_n) - P_h \varphi(t_n), \\ \xi_\sigma(t_n) &= (R_\sigma \varphi)(t_n) - \varphi_\sigma(t_n) = (R_\sigma \varphi)_{n+1,h} - \varphi_{n+1,h} \equiv \xi_{n+1,h}. \end{aligned}$$

For $n = N$, $(R_\sigma \varphi)_{N+1,h} = P_h \varphi(T)$ and $\varphi_{N+1,h} = \gamma(y_{N,h} - y_{\Omega,h})$. From (5.16) and (6.44), we deduce for each $n = N, \dots, 1$, and for all $w_h \in Y_h$, that

$$\begin{aligned} &(e(t_{n-1}) - e(t_n), w_h) + \int_{t_{n-1}}^{t_n} (\nabla e(t), \nabla w_h) dt + \epsilon^{-2} \int_{t_{n-1}}^{t_n} ((3y^2 - 1)\varphi, w_h) dt \\ &- \epsilon^{-2} \int_{t_{n-1}}^{t_n} ((3y_{n,h}^2 - 1)\varphi_{n,h}, w_h) dt = \int_{t_{n-1}}^{t_n} (y(t) - y_{n,h}, w_h) dt. \end{aligned} \quad (6.65)$$

Setting $w_h = \xi_{n,h}$, using (6.64) and $(\eta(t_n), \xi_{n,h}) = 0$, and adding and subtracting appropriate terms, (6.65) yields,

$$\begin{aligned} &(\xi_{n,h} - \xi_{n+1,h}, \xi_{n,h}) + \int_{t_{n-1}}^{t_n} \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 dt \\ &+ 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} ((y^2 - y_\sigma^2)\varphi_{n,h}, \xi_{n,h}) dt + \epsilon^{-2} \int_{t_{n-1}}^{t_n} ((3y^2 - 1)(\varphi - \varphi_{n,h}), \xi_{n,h}) dt \\ &= \int_{t_{n-1}}^{t_n} (y - y_\sigma, \xi_{n,h}) dt - \int_{t_{n-1}}^{t_n} (\nabla \eta, \nabla \xi_{n,h}) dt. \end{aligned}$$

Relation (6.64), and standard algebraic manipulations imply that

$$\begin{aligned}
& \frac{1}{2} \|\xi_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|\xi_{n+1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\xi_{n,h} - \xi_{n+1,h}\|_{L_2(\Omega)}^2 \\
& + \int_{t_{n-1}}^{t_n} \left(\|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 + \epsilon^{-2} ((3y^2 - 1)\xi_{n,h}, \xi_{n,h}) \right) dt \\
& = \int_{t_{n-1}}^{t_n} (y - y_\sigma, \xi_{n,h}) dt - \int_{t_{n-1}}^{t_n} (\nabla \eta, \nabla \xi_{n,h}) dt \\
& - 3\epsilon^{-2} \int_{t_{n-1}}^{t_n} ((y - y_\sigma)(y_\sigma + y)\varphi_{n,h}, \xi_{n,h}) dt \\
& - \epsilon^{-2} \int_{t_{n-1}}^{t_n} ((3y^2 - 1)\eta, \xi_{n,h}) dt \\
& := \sum_{j=1}^4 \mathcal{T}_j.
\end{aligned}$$

Applying Hölder and Young's inequalities, we easily get

$$\begin{aligned}
\mathcal{T}_1 & \leq \frac{1}{2} \int_{t_{n-1}}^{t_n} \|y - y_\sigma\|_{L_2(\Omega)}^2 dt + \frac{1}{2} \int_{t_{n-1}}^{t_n} \|\xi_{n,h}\|_{L_2(\Omega)}^2 dt, \\
\mathcal{T}_2 & \leq \frac{1}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|\nabla \eta\|_{L_2(\Omega)}^2 dt + \frac{\epsilon^2}{4} \int_{t_{n-1}}^{t_n} \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 dt, \\
\mathcal{T}_4 & \leq \int_{t_{n-1}}^{t_n} \|y \xi_{n,h}\|_{L_2(\Omega)}^2 dt + \frac{1}{4\epsilon^4} \int_{t_{n-1}}^{t_n} \left(9\|y\|_{L_\infty(\Omega)}^2 + 1 \right) \|\eta\|_{L_2(\Omega)}^2 dt \\
& + \int_{t_{n-1}}^{t_n} \|\xi_{n,h}\|_{L_2(\Omega)}^2 dt.
\end{aligned}$$

We note that using Hölder and Young's inequalities, and the stability estimates of y, y_σ and φ_σ , we deduce

$$\begin{aligned}
\mathcal{T}_3 & \leq \frac{3}{\epsilon^2} \int_{t_{n-1}}^{t_n} \|y - y_\sigma\|_{L_2(\Omega)} \|\varphi_{n,h}\|_{L_6(\Omega)} \left(\|y_\sigma\|_{L_6(\Omega)} + \|y\|_{L_6(\Omega)} \right) \|\xi_{n,h}\|_{L_6(\Omega)} dt \\
& \leq \frac{9C(C_{st,2} + C_{st,2}^{dG})^2}{\epsilon^6} \int_{t_{n-1}}^{t_n} \|y - y_\sigma\|_{L_2(\Omega)}^2 \|\varphi_{n,h}\|_{L_6(\Omega)}^2 dt \\
& + \frac{\epsilon^2}{4} \int_{t_{n-1}}^{t_n} \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 dt, \\
& \leq \frac{9C(C_{st,2} + C_{st,2}^{dG})^2}{\epsilon^6} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 \int_{t_{n-1}}^{t_n} \|\varphi_{n,h}\|_{L_6(\Omega)}^2 dt \\
& + \frac{\epsilon^2}{4} \int_{t_{n-1}}^{t_n} \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 dt,
\end{aligned}$$

where C is a constant depending only on the domain. Using the spectral estimate at

'continuous level' (3.20) for $v = \xi_{n,h}$ and collecting the above bounds, we have

$$\begin{aligned} & \frac{1}{2} \|\xi_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|\xi_{n+1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\xi_{n,h} - \xi_{n+1,h}\|_{L_2(\Omega)}^2 \\ & + \frac{\epsilon^2}{2} \int_{t_{n-1}}^{t_n} \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 dt + 2 \int_{t_{n-1}}^{t_n} \|y \xi_{n,h}\|_{L_2(\Omega)}^2 dt \\ & \leq \int_{t_{n-1}}^{t_n} \left(\frac{9\|y\|_{L_\infty(\Omega)}^2 + 1}{4\epsilon^4} \|\eta\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} \|\nabla \eta\|_{L_2(\Omega)}^2 \right) dt + \frac{1}{2} \int_{t_{n-1}}^{t_n} \|y - y_\sigma\|_{L_2(\Omega)}^2 dt \\ & + \frac{9C(C_{st,2} + C_{st,2}^{dG})^2}{\epsilon^6} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 \int_{t_{n-1}}^{t_n} \|\varphi_{n,h}\|_{L_6(\Omega)}^2 dt \\ & + \int_{t_{n-1}}^{t_n} \left(\lambda(t)(1 - \epsilon^2) + \frac{5}{2} \right) \|\xi_{n,h}\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

Summing from $n = m$ up to N where $1 \leq m \leq N$, using a standard (linear) Gronwall Lemma, for $\sup_{n=1,\dots,N} \alpha k_n < 1$, where $\alpha := \sup_{t \in [0,T]} (2\lambda(t)(1 - \epsilon^2) + 5)$, we deduce

$$\begin{aligned} & \|\xi_{m,h}\|_{L_2(\Omega)}^2 + \sum_{n=m}^N \|\xi_{n,h} - \xi_{n+1,h}\|_{L_2(\Omega)}^2 + \epsilon^2 \sum_{n=m}^N k_n \|\nabla \xi_{n,h}\|_{L_2(\Omega)}^2 \\ & \leq E \left\{ \|\xi_{N+1,h}\|_{L_2(\Omega)}^2 + \int_{t_m}^T \left(\frac{9\|y\|_{L_\infty(\Omega)}^2 + 1}{2\epsilon^4} \|\eta\|_{L_2(\Omega)}^2 + \frac{2}{\epsilon^2} \|\nabla \eta\|_{L_2(\Omega)}^2 \right) dt \right. \\ & \quad + \frac{C(C_{st,2} + C_{st,2}^{dG})^2}{\epsilon^6} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 \int_{t_m}^T \|\varphi_\sigma\|_{L_6(\Omega)}^2 dt \\ & \quad \left. + \int_{t_m}^T \|y - y_\sigma\|_{L_2(\Omega)}^2 dt \right\}, \end{aligned}$$

with $E := \exp(T\alpha)$. Note that $C_{st,2} \sim 1/\epsilon$ and $C_{st,2}^{dG} \sim 1/\epsilon$. The estimate follows using the embedding $H^1(\Omega) \subset L_6(\Omega)$ and Lemma 6.12 to bound $\int_{t_m}^T \|\varphi_\sigma\|_{L_6(\Omega)}^2 dt \leq (D_{st,1}^{dG}/\epsilon)^2$ and Remark 6.8 to bound

$$\begin{aligned} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 & \leq \frac{C}{\epsilon^{2r}} (\kappa + h^2) \quad \text{for } d = 2, \\ \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))}^2 & \leq \frac{C}{\epsilon^{(7r-1)/3}} (\kappa + h^2) \quad \text{for } d = 3 \end{aligned}$$

Note that the term $\frac{2}{\epsilon^2} \int_{t_m}^T \|\nabla \eta\|_{L_2(\Omega)}^2 \leq \frac{C}{\epsilon^2} (k + h^2) \|\phi\|_{H^{2,1}(\Omega_T)}^2$ dominates all η terms. \square

The following result is analogous to Corollary 6.10 and an immediate consequence of Theorem 6.13, Lemma 5.10.

Corollary 6.14. Let $u, v \in L_2(0, T; L_2(\Omega))$ and $\varphi_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ be the solution of (5.16) while $\varphi_\sigma(v) \in Y_\sigma$ the solution of (6.44) corresponding to the control v . Assume that Lemmas 5.10 and 6.12 and Theorem 6.13 hold and let $r \in \{1, 2\}$. Then, for $d = 2$ there holds

$$\begin{aligned} & \|\varphi_u - \varphi_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi_u - \varphi_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \frac{L_2}{\epsilon^{7/2}} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{5+r}}, \end{aligned} \tag{6.66}$$

while for $d = 3$ it follows that

$$\begin{aligned} & \|\varphi_u - \varphi_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi_u - \varphi_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \frac{L_3}{\epsilon^{15/4}} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{5+(7r-1)/6}}; \end{aligned} \quad (6.67)$$

here, in line with the notation of Lemma 5.10 we set

$$\begin{aligned} L_2 &:= L_1 \left(\epsilon^{7/2} C_T E_\varphi^{1/2} + \tilde{c} C_\infty^{1/2} D_{st,1} \right), \\ L_3 &:= L_1 \left(\epsilon^{15/4} C_T E_\varphi^{1/2} + \tilde{c} C_\infty^{1/2} D_{st,1} \right). \end{aligned} \quad (6.68)$$

Proof. The estimate follows by triangle inequality. \square

6.2 Convergence of the discrete control problem

In this section we study the convergence of solutions of the discrete control problem (6.5) towards solutions of the continuous problem (5.3). Every discrete problem (6.5) has at least one solution because the minimization function is continuous and coercive on a nonempty closed subset of a finite dimensional space.

Theorem 6.15. For every $\sigma = (k, h)$, let \bar{u}_σ be a global solution of problem (6.5). Then, the sequence $\{\bar{u}_\sigma\}_\sigma$ is bounded in $L_2(0, T; L_2(\Omega))$ and there exist subsequences denoted in the same way, converging to a point \bar{u} weakly in $L_2(0, T; L_2(\Omega))$. Any of these limit points is a solution of problem (5.3). Moreover, we have

$$\lim_{\sigma \rightarrow 0} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} = 0 \quad \text{and} \quad \lim_{\sigma \rightarrow 0} J_\sigma(\bar{u}_\sigma) = J(\bar{u}). \quad (6.69)$$

The next theorem is important from a practical point of view because it states that every strict local minimum of problem (5.3) can be approximated by local minima of problems (6.5).

Theorem 6.16. Let \bar{u} be a strict local minimum of (5.3). Then, there exists a sequence $\{\bar{u}_\sigma\}_\sigma$ of local minima of problems (6.5) such that (6.69) holds.

Both proofs of the above Theorems are presented in detail in [CC12, Theorems 4.15 and 4.17].

Remark 6.17. It is important to mention that in our case, the above convergence results are proved for each fixed interface length, ϵ .

6.2.1 Error estimates

In this section we denote by \bar{u} a local solution of (5.3) and \bar{u}_σ a local solution of (6.5) for each σ . From Theorems 6.15 and 6.16, we deduce that $\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$. Moreover, let \bar{y} and $\bar{\varphi}$ be the state and the adjoint state associated to \bar{u} while \bar{y}_σ and $\bar{\varphi}_\sigma$ the discrete state and adjoint state corresponding to \bar{u}_σ .

Definition 6.18. We denote by u_σ the $L_2(0, T; L_2(\Omega))$ -projection of \bar{u} into U_σ defined through,

$$u_\sigma = \sum_{n=1}^N \sum_{\tau \in \mathcal{T}_h} u_{n,\tau} \chi_n \chi_\tau \quad \text{where} \quad u_{n,\tau} = \frac{1}{k_n |\tau|} \int_{t_{n-1}}^{t_n} \int_\tau |\bar{u}(t, x)| \, dx \, dt. \quad (6.70)$$

Lemma 6.19. Let $\bar{u} \in H^1(\Omega_T)$. Then, there exists constant $C > 0$ independent of $\sigma = (k, h)$ and ϵ , such that

$$\|\bar{u} - u_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq C(\sqrt{k} + h)\|\bar{u}\|_{H^1(\Omega_T)}, \quad (6.71)$$

$$\|\bar{u} - u_\sigma\|_{H^{-1}(\Omega_T)} \leq C(k + h^2) \|\bar{u}\|_{H^1(\Omega_T)}. \quad (6.72)$$

Proof. The estimate in the $L_2(0, T; L_2(\Omega))$ -norm is known. Let $v \in H^1(\Omega_T)$ and $v_\sigma \in U_\sigma$ defined as in (6.70). Then,

$$\begin{aligned} \int_0^T \int_\Omega v(\bar{u} - u_\sigma) dx dt &= \int_0^T \int_\Omega (v - v_\sigma)(\bar{u} - u_\sigma) dx dt \\ &\leq \|v - v_\sigma\|_{L_2(0,T;L_2(\Omega))} \|\bar{u} - u_\sigma\|_{L_2(0,T;L_2(\Omega))} \\ &\leq Ch^2 \|v\|_{H^1(\Omega_T)} \|\bar{u}\|_{H^1(\Omega_T)}, \end{aligned}$$

which completes the proof. \square

Theorem 6.20. Suppose that the assumptions of Theorems 5.11 and 5.13 and Corollaries 6.10 and 6.14 hold. Then, there exist $\mathcal{C} := \sqrt{T}\hat{C}$, $\tilde{\mathcal{C}} = L_1\mathcal{C}$ such that, for $d = 2$ and $r = 1, 2$, we have

$$\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq \frac{\mathcal{C}}{\epsilon^{5+r}} (\sqrt{k} + h), \quad (6.73)$$

$$\|\bar{y} - \bar{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\bar{y} - \bar{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{\tilde{\mathcal{C}}}{\epsilon^{5+r}} (\sqrt{k} + h). \quad (6.74)$$

In addition, for $d = 3$ and $r = 1, 2$ there holds

$$\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq \frac{\mathcal{C}}{\epsilon^{5+(7r-1)/6}} (\sqrt{k} + h), \quad (6.75)$$

$$\|\bar{y} - \bar{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\bar{y} - \bar{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{\tilde{\mathcal{C}}}{\epsilon^{5+(7r-1)/6}} (\sqrt{k} + h). \quad (6.76)$$

Proof. (Sketch:) The proof follows as in [CC12, Section 4]. We begin with $d = 3$. Note that (6.76) is a consequence of (6.75) combined with (6.39) and (6.40). Thus, the main subject is the proof of (6.75). Suppose that (6.75) is false. Specifically, this assumption implies that

$$\limsup_{\sigma \rightarrow 0} \frac{\epsilon^{5+(7r-1)/6}}{\mathcal{C}(\sqrt{k} + h)} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} = +\infty.$$

This means that there exists a sequence of σ such that

$$\lim_{\sigma \rightarrow 0} \frac{\epsilon^{5+(7r-1)/6}}{\mathcal{C}(\sqrt{k} + h)} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} = +\infty. \quad (6.77)$$

We aim to conclude to a contradiction. First of all, the fact that \bar{u}_σ is a local minimum of (6.5) combined with the property that J_σ is of class C^∞ and $u_\sigma \in U_{\sigma,ad}$ imply that $J'_\sigma(\bar{u}_\sigma)(u_\sigma - \bar{u}_\sigma) \geq 0$. After basic manipulations, the last inequality can be written in the form

$$\begin{aligned} J'(\bar{u}_\sigma)(\bar{u} - \bar{u}_\sigma) + [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u}_\sigma)](\bar{u} - \bar{u}_\sigma) \\ + [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u})](u_\sigma - \bar{u}) + J'(\bar{u})(u_\sigma - \bar{u}) \geq 0. \end{aligned}$$

Since \bar{u} is an local minimum of (5.3) and $\bar{u}_\sigma \in U_{ad}$, then $J'(\bar{u})(\bar{u}_\sigma - \bar{u}) \geq 0$. Adding this nonnegative term to the above inequality, it yields that

$$\begin{aligned} [J'(\bar{u}_\sigma) - J'(\bar{u})](\bar{u}_\sigma - \bar{u}) &\leq [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u}_\sigma)](\bar{u} - \bar{u}_\sigma) \\ &+ [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u})](u_\sigma - \bar{u}) + J'(\bar{u})(u_\sigma - \bar{u}). \end{aligned} \quad (6.78)$$

We shall derive an estimate from below for the left-hand side and then an upper bound for the three terms on the right-hand side of the above inequality. To do so, we consider a sequence $\{\bar{u}_\sigma\}_\sigma$ that satisfies (6.77). The property that J is of class C^∞ combined with the Mean Value Theorem imply that for some $\hat{u}_\sigma = \bar{u} + \theta_h(\bar{u}_\sigma - \bar{u})$ it holds that

$$[J'(\bar{u}_\sigma) - J'(\bar{u})](\bar{u}_\sigma - \bar{u}) = J''(\hat{u}_\sigma)(\bar{u}_\sigma - \bar{u})^2. \quad (6.79)$$

We define

$$v_\sigma = \frac{1}{\rho_\sigma}(\bar{u}_\sigma - \bar{u}) \quad \text{where} \quad \rho_\sigma = \|\bar{u}_\sigma - \bar{u}\|_{L_2(0,T;L_2(\Omega))},$$

and take a subsequence such that $v_\sigma \rightharpoonup v$ in $L_2(0,T;L_2(\Omega))$, if it is necessary. Note that v_σ satisfies the sign conditions *ii*) – *iii*) of critical cone $C_{\bar{u}}$ by construction. Indeed, since $\bar{u} \in U_{ad}$ we obtain that

$$\begin{cases} \text{if } \bar{u}(t,x) = u_a \text{ then } v_\sigma = \frac{1}{\rho_\sigma}(\bar{u}_\sigma - u_a) \geq 0, \\ \text{if } \bar{u}(t,x) = u_b \text{ then } v_\sigma = \frac{1}{\rho_\sigma}(\bar{u}_\sigma - u_b) \leq 0. \end{cases}$$

Hence v also satisfies the sign conditions *ii*) – *iii*) of critical cone $C_{\bar{u}}$. Thus, it remains to show that the first condition of the critical cone,

$$v(t,x) = 0 \quad \text{if} \quad \bar{d}(t,x) = \bar{\varphi}(t,x) + \mu\bar{u}(t,x) \neq 0,$$

is satisfied. For brevity, we denote by

$$\bar{d}_\sigma = \bar{\varphi}_\sigma + \mu\bar{u}_\sigma.$$

From Theorems 6.15 and 6.16, we deduce that $\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$, since \bar{u}_σ is a local minimum of (6.5) while \bar{u} is an local minimum of (5.3). This convergence result together with (6.67) implies that, as $\sigma \rightarrow 0$,

$$\|\bar{d} - \bar{d}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0.$$

Thus, we have that

$$\begin{aligned} \int_0^T \int_\Omega \bar{d}v \, dx \, dt &= \lim_{\sigma \rightarrow 0} \int_0^T \int_\Omega \bar{d}_\sigma v_\sigma \, dx \, dt \\ &= \lim_{\sigma \rightarrow 0} \frac{1}{\rho_\sigma} \left\{ \int_0^T \int_\Omega \bar{d}_\sigma(u_\sigma - \bar{u}) \, dx \, dt + \int_0^T \int_\Omega \bar{d}_\sigma(\bar{u}_\sigma - u_\sigma) \, dx \, dt \right\}. \end{aligned}$$

Using the inequality $J'_\sigma(\bar{u}_\sigma)(\bar{u}_\sigma - u_\sigma) \leq 0$ and (6.77), (6.71), we deduce that

$$\begin{aligned} \int_0^T \int_\Omega \bar{d}v \, dx \, dt &\leq \lim_{\sigma \rightarrow 0} \frac{1}{\rho_\sigma} \int_0^T \int_\Omega \bar{d}_\sigma(u_\sigma - \bar{u}) \, dx \, dt \\ &\leq \lim_{\sigma \rightarrow 0} \frac{C(\sqrt{k} + h)\|\bar{u}\|_{H^1(\Omega_T)}}{\|\bar{u}_\sigma - \bar{u}\|_{L_2(0,T;L_2(\Omega))}} = 0. \end{aligned}$$

We have already shown that v satisfies the sign conditions *ii) – iii)* of the critical cone $C_{\bar{u}}$, then $\bar{d}(t, x)v(t, x) \geq 0$. Hence the above inequality implies that the first condition of $C_{\bar{u}}$ holds as well, then $v \in C_{\bar{u}}$.

Now, from (5.15) and the definition of v_σ

$$\begin{aligned} J''(\hat{u}_\sigma)v_\sigma^2 &= \int_0^T \int_\Omega |z_{v_\sigma}|^2 dx dt + \gamma \int_\Omega |z_{v_\sigma}(T)|^2 dx \\ &\quad - 6\epsilon^{-2} \int_0^T \int_\Omega y_{\hat{u}_\sigma} z_{v_\sigma}^2 \varphi_{\hat{u}_\sigma} dx dt + \mu. \end{aligned}$$

From the definition of \hat{u}_σ and the fact that $\|\bar{u} - \hat{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$, we deduce that $\hat{u}_\sigma \rightarrow \bar{u}$ in $L_2(0, T; L_2(\Omega))$ strongly. Furthermore, $z_{v_\sigma} \rightharpoonup z_v$ in $H^{2,1}(\Omega_T)$ while $y_{\hat{u}_\sigma} \rightarrow \bar{y}$ and $\varphi_{\hat{u}_\sigma} \rightarrow \bar{\varphi}$ in $H^{2,1}(\Omega_T)$. Then, passing the limit and recalling the equivalent second order sufficient condition (5.44), we get that

$$\begin{aligned} &\lim_{\sigma \rightarrow 0} J''(\hat{u}_\sigma)v_\sigma^2 \\ &= \lim_{\sigma \rightarrow 0} \left\{ \int_0^T \int_\Omega |z_{v_\sigma}|^2 dx dt + \gamma \int_\Omega |z_{v_\sigma}(T)|^2 dx - 6\epsilon^{-2} \int_0^T \int_\Omega y_{\hat{u}_\sigma} z_{v_\sigma}^2 \varphi_{\hat{u}_\sigma} dx dt + \mu \right\} \\ &= \int_0^T \int_\Omega |z_v|^2 dx dt + \gamma \int_\Omega |z_v(T)|^2 dx - 6\epsilon^{-2} \int_0^T \int_\Omega \bar{y} z_v^2 \bar{\varphi} dx dt + \mu \\ &= J''(\bar{u})v^2 + \mu \left(1 - \|v\|_{L_2(0,T;L_2(\Omega))}^2 \right) \\ &\geq \mu + (\delta - \mu) \|v\|_{L_2(0,T;L_2(\Omega))}^2. \end{aligned}$$

Taking into account $\|v\|_{L_2(0,T;L_2(\Omega))} \leq 1$, these inequalities lead to

$$\lim_{\sigma \rightarrow 0} J''(\hat{u}_\sigma)v_\sigma^2 \geq \min\{\delta, \mu\} > 0,$$

which proves the existence of σ_0 , with $|\sigma| > 0$, such that

$$J''(\hat{u}_\sigma)v_\sigma^2 \geq \frac{1}{2} \min\{\delta, \mu\} > 0, \quad \forall |\sigma| < |\sigma_0|.$$

From the above inequality and the definition of v_σ , (6.79) becomes,

$$\frac{1}{2} \min\{\delta, \mu\} \|\bar{u}_\sigma - \bar{u}\|_{L_2(0,T;L_2(\Omega))}^2 \leq [J'(\bar{u}_\sigma) - J'(\bar{u})](\bar{u}_\sigma - \bar{u}) \quad \text{if } |\sigma| < |\sigma_0|.$$

Inserting the above lower bound in (6.78) we obtain that,

$$\begin{aligned} &\frac{1}{2} \min\{\delta, \lambda\} \|\bar{u}_\sigma - \bar{u}\|_{L_2(0,T;L_2(\Omega))}^2 \leq [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u}_\sigma)](\bar{u} - \bar{u}_\sigma) \\ &\quad + [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u})](\bar{u}_\sigma - \bar{u}) + J'(\bar{u})(\bar{u}_\sigma - \bar{u}). \end{aligned} \tag{6.80}$$

We shall estimate from above the three terms on the right-hand side of (6.80). More specifically, from (5.14) and (6.45), we have

$$\begin{aligned} &[J'_\sigma(\bar{u}_\sigma) - J'(\bar{u}_\sigma)](\bar{u} - \bar{u}_\sigma) \\ &\leq \|\bar{\varphi}_\sigma - \varphi_{\bar{u}_\sigma}\|_{L_2(0,T;L_2(\Omega))} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \\ &\leq \sqrt{T} \|\bar{\varphi}_\sigma - \varphi_{\bar{u}_\sigma}\|_{L_\infty(0,T;L_2(\Omega))} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \\ &\leq \frac{\sqrt{T} \hat{C}}{\epsilon^{5+(7r-1)/6}} (\sqrt{k} + h) \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))}, \end{aligned} \tag{6.81}$$

using the estimate (6.67) for $u = v = \bar{u}_\sigma$. For the second term on the right-hand side of (6.80), we recall again (6.67) for $u = \bar{u}$ and $v = \bar{u}_\sigma$ and (6.71), to get

$$\begin{aligned} & [J'_\sigma(\bar{u}_\sigma) - J'(\bar{u})](u_\sigma - \bar{u}) \\ & \leq \left(\|\bar{\varphi}_\sigma - \bar{\varphi}\|_{L_2(0,T;L_2(\Omega))} + \mu \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \right) \|u_\sigma - \bar{u}\|_{L_2(0,T;L_2(\Omega))} \\ & \leq C \left\{ \left(\frac{\sqrt{T}L_3}{\epsilon^{15/4}} + \mu \right) \|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \right. \\ & \quad \left. + \frac{\sqrt{T}\hat{C}}{\epsilon^{5+(7r-1)/6}} (\sqrt{k} + h) \right\} (\sqrt{k} + h) \|\bar{u}\|_{H^1(\Omega_T)}. \end{aligned} \quad (6.82)$$

Finally, using (5.28) to bound $\|\bar{\varphi} + \mu\bar{u}\|_{H^1(\Omega_T)} \leq C\|\bar{\varphi}\|_{H^1(\Omega_T)}$ and (6.72) we have

$$\begin{aligned} & J'(\bar{u})(u_\sigma - \bar{u}) \\ & \leq \|\bar{\varphi} + \mu\bar{u}\|_{H^1(\Omega_T)} \|u_\sigma - \bar{u}\|_{H^{-1}(\Omega_T)} \\ & \leq C(k + h^2) \|\bar{u}\|_{H^1(\Omega_T)} \|\bar{\varphi}\|_{H^1(\Omega_T)}. \end{aligned} \quad (6.83)$$

Applying Young's inequality on the right-hand side of (6.81), (6.82), (6.83) and collecting the terms properly in (6.80), we derive

$$\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq \max \left\{ \frac{\sqrt{T}L_3}{\epsilon^{15/4}} \|\bar{u}\|_{H^1(\Omega_T)}, \frac{\sqrt{T}\hat{C}}{\epsilon^{5+(7r-1)/6}} \right\} (\sqrt{k} + h).$$

We note that from (5.28) and Theorem 5.11 we have that $\|\bar{u}\|_{H^1(\Omega_T)} \sim \epsilon^{-2}$ hence for $r = 1, 2$ the second term dominates the maximum. Hence, we deduce the desired estimate (6.75) for $C = \sqrt{T}\hat{C}$. For the proof of (6.76), we recall (6.39) and (6.40) for $u = \bar{u}, v = \bar{u}_\sigma$ combined with (6.75). The proof of $d = 2$ -case results upon arguing in the same way. \square

Theorem 6.20 is the conclusive result of both Chapters 5 and 6. It is evident from the hypotheses of the final theorem that we should combine all the results in order to establish the desired estimates for the difference between local optimal controls and their discrete approximations, as well as estimates for the differences between the corresponding state and adjoint state and their discrete approximations. The aim of our approach is the derivation of estimates with bounding constants that depend on $1/\epsilon$ only polynomially, while the conditional assumptions on the mesh-size parameters $\sigma = (h, k)$ and the interface length exhibit a favorable dependence. This justifies our interest in the $1/\epsilon$ -dependence of Lipschitz constants in the proofs of the Lipschitz continuity of the control to state and the state to adjoint mappings. The error analysis of both state and adjoint state equations require a lot of technical arguments throughout the proofs to avoid the construction of a discrete approximation of the spectral estimate; the latter is incompatible to the regularity imposed of the optimal control setting.

CHAPTER 7

FUTURE WORK

We shall now discuss some aspects of further research that arise naturally. A significant undertaking topic is the use within adaptive algorithms of the conditional type *a posteriori* error estimators that were proven in our first work [CGP20], Chapter 3. Seeking to prove *a posteriori* error estimates for the $L_4(0, T; L_4(\Omega))$ -norm is, in our view, justified, as they can be potentially used to drive space-time adaptive algorithms without excessive proliferation of numerical degrees of freedom. As a result, the design of space-time adaptive algorithms for the proposed backward Euler in time combined with conforming finite element method in space could verify the practical reliance of the analysis. Additionally, we have pointed out that the new *a posteriori* error analysis appears to improve the ϵ -dependence on the conditional-assumptions for $L_2(0, T; H^1(\Omega))$ - and $L_\infty(0, T; L_2(\Omega))$ -norms bounds compared to previous works of [FW05, Bar05, BMO11, BM11] in certain cases. Of course, it is clear that the performance of the proposed estimates above has to be assessed numerically before any conclusive statements can be made.

The analysis of Chapter 4, is devoted to the derivation of conditional type *a posteriori* error estimates for the fully-discrete DG-IPDG finite element approximations of the Allen-Cahn equation on general polytopic meshes. The implementation of the above algorithms is both interesting and challenging project itself and it is in preparation. Going one step further, the exploitation of DG-IPDG method using polynomial spaces defined in the physical frame naturally allows for the use of computational meshes consisting of general polytopic elements. General shaped elements offer great flexibility in practical computations and reduce the computational cost for mesh refinement and coarsening. The resolution of time-dependent sharp *interfaces* remains a challenge in the quest of resolved computations. Mesh-geometry freedom, in conjunction with variable order local polynomial elemental degrees, is expected to achieve accurate approximation while simultaneously reduces the sizes of the resulting systems required to be solved per time-step.

The new *a posteriori* error analysis of the Allen-Cahn problem presented in Chapters 3 and 4 appears to be applicable to the optimal control setting presented in Chapters 5 and 6. Indeed, we may begin with the the lowest order fully discrete scheme, backward Euler-finite element method (discontinuous in time dG(0) due to the low regularity imposed of the optimal control setting). With minor modifications only we

can directly apply the *a posteriori* estimates for the state solution. However, the main challenge is the derivation of (conditional or not) *a posteriori* error bounds of the corresponding discrete adjoint state equation (5.16). The suitable error approach in this case is still under investigation. The question is whether we will apply straightforward error techniques for parabolic PDEs comparing directly the difference between the approximation (6.44) and the exact solution (5.16), or is it more preferable to introduce the concept of splitting the total error through a suitably defined *space-time reconstruction*.

The adjoint state equation is a linearized around the state solution backward in time parabolic PDE. At first, we may assume that there is no need for a nonlinear Gronwall lemma (continuation argument). There are two key questions that we should take into account. Shall we study the error in the $L_4(0, T; L_4(\Omega))$ -norm? If we are interested in this direction, we need to construct a test function that will give rise to $L_4(0, T; L_4(\Omega))$ -norm since in contrast to the state equation (Allen-Cahn equation) it is not a norm arising naturally. How can we derive desired *a posteriori* error bounds that depend polynomially upon the inverse of the *interface* length $1/\epsilon$ without deducing additional conditional-assumption with higher ϵ -dependence compared to the analogous condition in the error analysis of the state problem?

As long as the *a posteriori* estimates of the adjoint state problem are available, they can be combined with the corresponding estimates of the state problem in order to deduce *a posteriori* bounds of the control error, $\bar{u} - \bar{u}_\sigma$. Again, the second order sufficient conditions would be the crucial connecting argument. Nonetheless, the latter is necessary to be reconsidered in order to be applicable in an *a posteriori* fashion around the discrete optimal control \bar{u}_σ .

If one is interested in measuring the control error in other norms except of the $L_2(0, T; L_2(\Omega))$ -norm, one should go back and recast the given optimal control problem. The first reasonable idea is to reconsider the energy functional or/and even the admissible set U_{ad} . Another possible scenario, according to the profile of the Allen-Cahn solution accross the the evolving interfaces, is the so called *bang-bang* control (for $\mu = 0$), where the values $\bar{u}(t, x)$ coincide almost everywhere with one of the thresholds values u_α or u_b .

In this vein, the study of other sophisticated examples of phase-field problems is also an interesting direction. More specifically, it is of independent interest to investigate whether the already proposed approximation schemes and the techniques used throughout this work could be transferred (maybe under some modifications) to Ginzburg-Landau, Cahn-Hilliard, Cahn-Larché equations. While many numerical methods designed for scalar equations can be extended to systems, there are new challenges associated with invariance and symmetries and choices of gauge [Du05] in addition to added computational complexity due to additional quantities of interests. The $L_4(0, T; L_4(\Omega))$ -focused theory presented in this work remains a possible starting point to investigate the aforementioned phase-field models due to the presence of the double-well potential.

CHAPTER

APPENDIX

A Proof of Lemma 6.4

We recall error representation (6.14),

$$\hat{e} = y - \hat{y}_\sigma = (y - P_\sigma y) + (P_\sigma y - \hat{y}_\sigma) = \hat{d} + \hat{e}_\sigma.$$

We are interested in bounding each term separately. More specifically, we already have estimated the so called projection error in Lemma 6.3. Thus, the main goal of this analysis is the estimation of \hat{e}_σ . Note that using the definition of L_2 -projection operator,

$$(\hat{d}(t_n) - \hat{d}(t_{n-1}), w_h) = (y(t_n) - P_h y(t_n), w_h) - (y(t_{n-1}) - P_h y(t_{n-1}), w_h) = 0$$

the identity (6.15) becomes

$$(\hat{e}_{n,h} - \hat{e}_{n-1,h}, w_h) + \int_{J_n} (\nabla \hat{e}_{n,h}, \nabla w_h) = - \int_{J_n} (\nabla \hat{d}, \nabla w_h), \quad (\text{A.1})$$

for all $w_h \in Y_h$ and for each $1 \leq n \leq N$. Putting $w_h = \hat{e}_{n,h}$,

$$\begin{aligned} & \frac{1}{2} \|\hat{e}_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|\hat{e}_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\hat{e}_{n,h} - \hat{e}_{n-1,h}\|_{L_2(\Omega)}^2 + k_n \|\nabla \hat{e}_{n,h}\|_{L_2(\Omega)}^2 \\ & \leq \frac{k_n}{2} \|\nabla \hat{e}_{n,h}\|_{L_2(\Omega)}^2 + \frac{k_n}{2} \|\nabla \hat{d}\|_{L_2(\Omega)}^2. \end{aligned}$$

Summing from $n = 1$ up to m where $1 \leq m \leq N$ to obtain that

$$\begin{aligned} & \|\hat{e}_{m,h}\|_{L_2(\Omega)}^2 + \sum_{n=1}^m \|\hat{e}_{n,h} - \hat{e}_{n-1,h}\|_{L_2(\Omega)}^2 + \int_0^{t_m} \|\nabla \hat{e}_{n,h}\|_{L_2(\Omega)}^2 dt \\ & \leq \|\hat{e}_{0,h}\|_{L_2(\Omega)}^2 + \int_0^{t_m} \|\nabla \hat{d}\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

Using the error representation (6.14) and the triangle inequality we deduce that

$$\begin{aligned} & \max_{1 \leq n \leq N} \|y(t_n) - \hat{y}_\sigma(t_n)\|_{L_2(\Omega)} + \|y - \hat{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq C \left(\sqrt{k} \|y_t\|_{L_2(0,T;L_2(\Omega))} + h \|y\|_{L_2(0,T;H^2(\Omega))} + h \|y_0\|_{H_0^1(\Omega)} \right). \end{aligned}$$

From the above estimate we are able to deduce an error estimate in $L_\infty(0, T; L_2(\Omega))$. Let assume that $t_{n-1} \leq t \leq t_n$ for some $n \leq N$,

$$\|y(t) - \hat{y}_\sigma(t)\|_{L_2(\Omega)} \leq \|y(t) - y(t_n)\|_{L_2(\Omega)} + \|y(t_n) - \hat{y}_\sigma(t_n)\|_{L_2(\Omega)}.$$

It remains to bound the first term, for any $v \in L_2(\Omega)$ we have that

$$\begin{aligned} |(y(t) - y(t_n), v)| &= \left| \left(\int_t^{t_n} y_t(s) \, ds, v \right) \right| \leq \int_t^{t_n} \|y_t(s)\|_{L_2(\Omega)} \, ds \|v\|_{L_2(\Omega)} \\ &\leq \sqrt{k} \|y_t\|_{L_2(0,T;L_2(\Omega))} \|v\|_{L_2(\Omega)}, \end{aligned}$$

which implies that

$$\|y(t) - y(t_n)\|_{L_2(\Omega)} \leq \sqrt{k} \|y_t\|_{L_2(0,T;L_2(\Omega))}.$$

Then, we deduce that

$$\begin{aligned} & \|y - \hat{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))} \\ & \leq C \left(\sqrt{k} \|y_t\|_{L_2(0,T;L_2(\Omega))} + h \|y\|_{L_2(0,T;H^2(\Omega))} + h \|y_0\|_{H_0^1(\Omega)} \right). \end{aligned}$$

Now, we proceed with the proof of the second approximation result (6.17) through a duality argument. We consider a backward in time parabolic equation with a suitable chosen right-hand side:

$$\begin{aligned} -z_t - \Delta z &= \hat{e}_\sigma && \text{in } \Omega_T \\ z &= 0 && \text{on } \partial\Omega \times (0, T), \\ z(T) &= 0 && \text{in } \Omega. \end{aligned}$$

The fully discrete scheme of the above problem within the discontinuous Galerkin time-stepping method takes the form: For each $n = N, \dots, 1$ and for all $z_h \in Y_h$,

$$\begin{aligned} & \left(\frac{z_{n,h} - z_{n+1,h}}{k_n}, w_h \right) + (\nabla z_{n,h}, \nabla w_h) = (\hat{e}_{n,h}, w_h), \\ & z_{N+1,h} = 0, \end{aligned} \tag{A.2}$$

We begin by computing $z_{N,h}$ using $z_{N+1,h}$ and then we descent from $n = N$ until $n = 1$. Note that we set $z_{n,h} = z_\sigma(t_{n-1})$, $1 \leq n \leq N$. Moreover, there holds the following estimate

$$\begin{aligned} \|z - z_h\| &\leq C \left(\sqrt{k} + h \right) \|z\|_{H^{2,1}(\Omega_T)} \\ &\leq C \left(\sqrt{k} + h \right) \|\hat{e}_\sigma\|_{L_2(0,T;L_2(\Omega))}, \end{aligned} \tag{A.3}$$

where we used the parabolic regularity.

Choosing $w_h = \hat{e}_{n,h}$ in (A.2) and $w_h = \hat{z}_{n,h}$ in (A.1), we obtain

$$(z_{n,h} - z_{n+1,h}, \hat{e}_{n,h}) + \int_{J_n} (\nabla z_{n,h}, \nabla \hat{e}_{n,h}) dt = \int_{J_n} \|\hat{e}_{n,h}\|_{L_2(\Omega)}^2 dt,$$

and

$$(\hat{e}_{n,h} - \hat{e}_{n-1,h}, z_h) + \int_{J_n} (\nabla \hat{e}_{n,h}, \nabla z_h) dt = - \int_{J_n} (\nabla \hat{d}, \nabla z_h) dt,$$

respectively. Subtracting the above two equalities, we get that

$$(z_{n,h} - z_{n+1,h}, \hat{e}_{n,h}) - (\hat{e}_{n,h} - \hat{e}_{n-1,h}, z_h) = \int_{J_n} \|\hat{e}_{n,h}\|_{L_2(\Omega)}^2 dt + \int_{J_n} (\nabla \hat{d}, \nabla z_h) dt.$$

Summing from $n = 1$ up to N and after some algebra,

$$\begin{aligned} & (\hat{e}_{0,h}, z_{n,h}) - (z_{N+1,h}, \hat{e}_{N,h}) = \int_0^T \|\hat{e}_{n,h}\|_{L_2(\Omega)}^2 dt + \int_0^T (\nabla \hat{d}, \nabla z_h) dt \\ &= \int_0^T \|\hat{e}_{n,h}\|_{L_2(\Omega)}^2 dt + \int_0^T (\nabla \hat{d}, \nabla (z_h - z)) dt + \int_0^T (\nabla \hat{d}, \nabla z) dt, \end{aligned}$$

where $z_{N+1,h} = 0$ and that $(\hat{e}_{0,h}, z_{n,h}) = (y_{0h} - P_h y_0, z_{n,h}) = 0$. Integrating the last term by parts in space and applying Cauchy-Schwarz inequality it yields that

$$\begin{aligned} & \int_0^T \|\hat{e}_\sigma\|_{L_2(\Omega)}^2 dt \\ & \leq \|\nabla \hat{d}\|_{L_2(0,T;L_2(\Omega))} \|\nabla(z - z_h)\|_{L_2(0,T;L_2(\Omega))} + \|\hat{d}\|_{L_2(0,T;L_2(\Omega))} \|\Delta z\|_{L_2(0,T;L_2(\Omega))} \\ & \leq C \|\nabla \hat{d}\|_{L_2(0,T;L_2(\Omega))} (\sqrt{k} + h) \|z\|_{H^{2,1}(\Omega_T)} \\ & \quad + C \|\hat{d}\|_{L_2(0,T;L_2(\Omega))} \left(\|z_t\|_{L_2(0,T;L_2(\Omega))} + \|\hat{e}_\sigma\|_{L_2(0,T;L_2(\Omega))} \right) \\ & \leq C \left(\|\nabla \hat{d}\|_{L_2(0,T;L_2(\Omega))} (\sqrt{k} + h) + \|\hat{d}\|_{L_2(0,T;L_2(\Omega))} \right) \|\hat{e}_\sigma\|_{L_2(0,T;L_2(\Omega))}. \end{aligned}$$

Finally, applying the estimates in Lemma 6.3 and through triangle inequality, we deduce the desired error bound,

$$\|y - \hat{y}_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq C \left(k \|y_t\|_{L_2(0,T;L_2(\Omega))} + h^2 \|y\|_{L_2(0,T;H^2(\Omega))} \right).$$

Now it remains to prove the stability result (6.18). To do so, we test (6.12) with $w_h = -\Delta_h \hat{y}_{n,h} \in Y_h$,

$$\begin{aligned} & \frac{1}{2} \|\nabla \hat{y}_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2} \|\nabla \hat{y}_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\nabla(\hat{y}_{n,h} - \hat{y}_{n-1,h})\|_{L_2(\Omega)}^2 \\ & k_n \|\Delta_h \hat{y}_{n,h}\|_{L_2(\Omega)}^2 = - \left(k_n \hat{f}_n, \Delta_h \hat{y}_{n,h} \right). \end{aligned} \tag{A.4}$$

Since $y(t) \in H^2(\Omega) \cap H_0^1(\Omega)$ for a.e. $t \in (0, T)$ and $\Delta_h \hat{y}_{n,h} \in Y_h \subset H_0^1(\Omega)$ we can integrate by parts with respect to space variable,

$$\begin{aligned} & - \left(k_n \hat{f}_n, \Delta_h \hat{y}_{n,h} \right) = - \int_{J_n} (y_t(t), \Delta_h \hat{y}_{n,h}) dt + \int_{J_n} (\Delta y, \Delta_h \hat{y}_{n,h}) dt \\ & \leq \int_{J_n} \|y\|_{H^2(\Omega)}^2 dt + \int_{J_n} \|y_t\|_{L_2(\Omega)}^2 dt + \frac{k_n}{2} \|\Delta_h \hat{y}_{n,h}\|_{L_2(\Omega)}^2. \end{aligned}$$

Substituting the above inequality into (A.4), it follows

$$\begin{aligned} \frac{1}{2}\|\nabla\hat{y}_{n,h}\|_{L_2(\Omega)}^2 - \frac{1}{2}\|\nabla\hat{y}_{n-1,h}\|_{L_2(\Omega)}^2 + \frac{1}{2}\|\nabla(\hat{y}_{n,h} - \hat{y}_{n-1,h})\|_{L_2(\Omega)}^2 \\ \frac{k_n}{2}\|\Delta_h\hat{y}_{n,h}\|_{L_2(\Omega)}^2 \leq \int_{J_n}\|y\|_{H^2(\Omega)}^2 dt + \int_{J_n}\|y_t\|_{L_2(\Omega)}^2 dt. \end{aligned}$$

Summing from $n = 1$ up to m where $1 \leq m \leq N$,

$$\|\nabla\hat{y}_{m,h}\|_{L_2(\Omega)}^2 \leq \|\nabla y_{0,h}\|_{L_2(\Omega)}^2 + 2 \int_0^T \|y\|_{H^2(\Omega)}^2 dt + 2 \int_0^T \|y_t\|_{L_2(\Omega)}^2 dt,$$

that proves the boundedness of $\{\hat{y}_\sigma\}_\sigma$ in $L_\infty(0, T; H_0^1(\Omega))$.

B Proof of Theorem 6.17

Let \tilde{u} be a solution of problem (5.3) and let us take u_σ defined by

$$u_\sigma = \sum_{n=1}^N \sum_{\tau \in \mathcal{T}_h} u_{n,\tau} \chi_n \chi_\tau \quad \text{with} \quad u_{n,\tau} = \frac{1}{k_n |\tau|} \int_{t_{n-1}}^{t_n} \int_\tau \tilde{u}(t, x) dx dt. \quad (\text{B.1})$$

Then, u_σ is the $L_2(0, T; L_2(\Omega))$ projection of \tilde{u} into U_σ and we obtain that as $\sigma \rightarrow 0$, $\|\tilde{u} - u_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$. Using Corollary 6.10, we easily deduce that $J_\sigma(u_\sigma) \rightarrow J(\tilde{u})$. On the other hand, it is immediate that $u_\sigma \in U_{\sigma,ad}$ for every σ , then the optimality of \bar{u}_σ , we have that

$$J_\sigma(\bar{u}_\sigma) \leq J_\sigma(u_\sigma) \quad \forall u_\sigma \in U_{\sigma,ad}.$$

By the definition of (6.6) and (B.1) we get

$$\frac{\mu}{2}\|\bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))}^2 \leq J_\sigma(\bar{u}_\sigma) \leq J_\sigma(u_\sigma) \leq C \quad \forall \sigma.$$

the above proves that $\{\bar{u}_\sigma\}_\sigma$ is bounded in $L_2(0, T; L_2(\Omega))$ for every σ . Therefore, we deduce the existence of subsequences weakly convergent. Let \bar{u} be one of these limit points. Obviously the property $\bar{u} \in U_{ad}$ holds. Moreover, using again Corollary 6.10 and the convexity of the cost functional in the third term involving the control, we have

$$\begin{aligned} \inf(5.3) &\leq J(\bar{u}) \leq \liminf_{\sigma \rightarrow 0} J_\sigma(\bar{u}_\sigma) \leq \limsup_{\sigma \rightarrow 0} J_\sigma(\bar{u}_\sigma) \\ &\leq \limsup_{\sigma \rightarrow 0} J_\sigma(u_\sigma) = J(\tilde{u}) = \inf(5.3), \end{aligned}$$

which implies that \bar{u} is a solution of (5.3) as well as the convergence $J_\sigma(\bar{u}_\sigma) \rightarrow J(\bar{u})$. From this convergence along with the convergence properties of $y_{\bar{u}_\sigma} \rightarrow y_{\bar{u}}$ given in Corollary 6.10, we get $\|\bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow \|\bar{u}\|_{L_2(0,T;L_2(\Omega))}$ and obtain strong convergence of $\{\bar{u}_\sigma\}_\sigma$ to \bar{u} .

C Proof of Theorem 6.18

Let \bar{u} be a strict local minimum of (5.3), then there exists $\alpha > 0$ such that \bar{u} is the unique solution of

$$\min_{u \in U_{ad} \cap \bar{B}_\alpha(\bar{u})} J(u), \quad (\text{C.1})$$

where $B_\alpha(\bar{u})$ is a ball in $L_2(0, T; L_2(\Omega))$.

Let us consider the discrete problems

$$\min_{u_\sigma \in U_{\sigma,ad} \cap \bar{B}_\alpha(\bar{u})} J_\sigma(u_\sigma). \quad (\text{C.2})$$

For every σ sufficiently small, the problem (C.2) has at least one solution. It remains to check that the set $U_{\sigma,ad} \cap \bar{B}_\alpha(\bar{u})$ is not empty. To this end, we define $u_\sigma \in U_{\sigma,ad} \cap \bar{B}_\alpha(\bar{u})$ as in (B.1), where \tilde{u} is replaced by \bar{u} . Then, $\|\bar{u} - u_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$, therefore $u_\sigma \in U_{\sigma,ad} \cap \bar{B}_\alpha(\bar{u})$ for every σ sufficiently small. Let \bar{u}_σ be a solution of (C.2). Then, we can argue as in the above proof to deduce that any subsequence of $\{\bar{u}_\sigma\}_\sigma$ converges strongly in $L_2(0, T; L_2(\Omega))$ to a solution of (C.1). Since this problem has a unique solution, we have that $\|\bar{u} - \bar{u}_\sigma\|_{L_2(0,T;L_2(\Omega))} \rightarrow 0$ for the whole sequence as $\sigma \rightarrow 0$. This implies that the constraint $\bar{u}_\sigma \in \bar{B}_\alpha(\bar{u})$ is not active for small σ and hence \bar{u}_σ is a local solution to (6.5) and (6.69) is fulfilled.

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Εκ των υστέρων ανάλυση σφάλματος και βέλτιστος έλεγχος για εξισώσεις πεδίου φάσεων

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Μάιος, 2022

CHAPTER

DETAILED ABSTRACT IN GREEK

A Εισαγωγή

Η ιδέα της μεθόδου του πεδίου φάσης μπορεί να αναχθεί στους Lord Rayleigh, Gibbs και Van der Waals και χρησιμοποιήθηκε για να περιγράψει τις διεπιφάνειες υλικών κατά τη διάρκεια αλλαγής φάσης. Συγκεκριμένα, αναπαριστά τις διεπιφάνειες υλικών ως λεπτά στρώματα πεπερασμένου πάχους κατά μήκος των οποίων οι ιδιότητες του κάθε υλικού πουκίλλουν. Το στρώμα αυτό συχνά αναφέρεται ως διεπιφάνεια διάχυσης και έχει σχεδιαστεί έτσι ώστε να διασφαλίζεται ότι η ακριβής διεπιφάνεια βρίσκεται μέσα σε αυτό το λεπτό στρώμα. Γι' αυτό το λόγο η μέθοδος πεδίου φάσης είναι επίσης γνωστή στη βιβλιογραφία με την ονομασία μέθοδος διάχυσης διεπιφανειών.

Η μέθοδος του πεδίου φάσης χρησιμοποιήθηκε αρχικά για τη μοντελοποίηση της αλλαγής φάσης στερεού-υγρού, όπου η επιφανειακή τάση και η μη ισορροπημένη θερμοδυναμική συμπεριφορά αποκτούν σημασία στη διεπιφάνεια. Τα τελευταία σαράντα χρόνια η μέθοδος του πεδίου φάσης έχει γίνει μια γενική μεθοδολογία για προβλήματα κινούμενης διεπιφάνειας που προκύπτουν από την αστροφυσική, τη βιολογία, τη διαφορική γεωμετρία, την επεξεργασία εικόνας, την πολυφασική ρευστομηχανική, τη χημική και πετρελαϊκή μηχανική, τη μετάβαση φάσης υλικών και τη στερεοποίηση. Το κοινό χαρακτηριστικό ενδιαφέρον στοιχείο των προαναφερθέντων προβλημάτων είναι η διεπιφανειακή ενέργεια η οποία παίζει καθοριστικό ρόλο σε κάθε μία από αυτές τις εξελίξεις της κινούμενης διεπιφάνειας. Από μαθηματική άποψη, οι διεπιφανειακές ενέργειες, η επιφανειακή τάση, χαρακτηρίζονται από τις καμπυλότητες της διεπιφάνειας, όπως για παράδειγμα την μέση ή την Gauss καμπυλότητα. Η μέθοδος του πεδίου φάσης αποδεικνύεται αποτελεσματική για τη μοντελοποίηση των ενεργειών της διεπιφάνειας, ιδίως του φαινομένου της επιφανειακής τάσης.

Τα προβλήματα διεπιφάνειας που εξελίσσονται υπό την επίδραση της επιφανειακής τάσης ή διεπιφανειακής ενέργειας ανήκουν στην κατηγορία των λεγόμενων γεωμετρικά κινούμενων προβλημάτων διεπιφάνειας. Η κίνηση εξελίσσεται σύμφωνα με κάποιο γεωμετρικό νόμο που εξαρτάται από την καμπυλότητα και καθορίζει την ταχύτητα V ή την κανονική ταχύτητα V_n των σημείων της διεπιφάνειας σε κάθε δεδομένη χρονική στιγμή t . Η διατύπωση του πεδίου φάσης αυτών

των προβλημάτων οδηγεί σε ενδιαφέρουσες και απαιτητικές μερικές διαφορικές εξισώσεις (ΜΔΕ). Ένα από τα πιο γνωστά γεωμετρικά προβλήματα κινούμενης διεπιφάνειας είναι η ροή μέσης καμπυλότητας της οποίας ο γεωμετρικός νόμος που διέπει είναι:

$$V \cdot n = H_{\Gamma_t},$$

όπου n το προς τα έξω κάθετο διάνυσμα στην κινούμενη διεπιφάνεια Γ_t , ενώ H_{Γ_t} συμβολίζουμε τη μέση καμπυλότητα. Για μια πρόσφατη ολοκληρωμένη ανασκόπηση των μοντέλων πεδίου φάσεων και της σχέσης τους με τις γεωμετρικές ροές, αναφερόμαστε στην [DF20].

Είναι γνωστό ότι η διατύπωση του πεδίου φάσης της ροής μέσης καμπυλότητας είναι η εξίσωση Allen-Cahn: Αναζητούμε $u : (0, T] \times \Omega \rightarrow \mathbb{R}$ τέτοια ώστε

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

Η εξίσωση αυτή εισήχθη αρχικά από τους Samuel M. Allen και John W. Cahn [AC79] για να περιγράψει την έννοια των συνόρων στα κρυσταλλικά στερεά. Προτάθηκε ως ένα απλό μοντέλο για τη διαδικασία του διαχωρισμού φάσεων ενός δυαδικού κράματος σε σταθερή θερμοκρασία. Η συνοριακή συνθήκη υποδηλώνει ότι δεν εμφανίζεται μάζα πέρα από τα τοιχώματα του δοχείου Ω . Να σημειώσουμε ότι διαφέρει από την αρχική εξίσωση Allen-Cahn στην κλιμάκωση του χρόνου, δηλαδή το t εδώ, που ονομάζεται ο γρήγορος χρόνος, αντιτροσωπεύει t/ϵ^2 στην αρχική διατύπωση. Εκεί, η συνάρτηση u αντιτροσωπεύει τη συγκέντρωση ενός από τα δύο μεταλλικών συστατικών του κράματος.

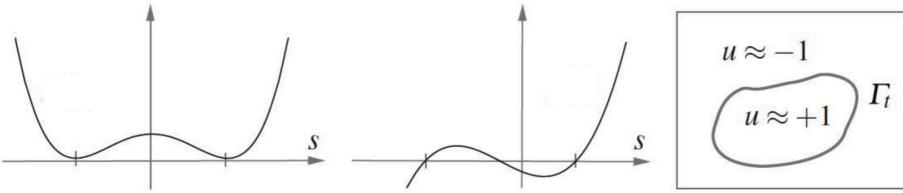
Η μη γραμμική συνάρτηση $F(s) := s^3 - s$ είναι η παράγωγος του κλασικού διπλού δυναμικού $\mathcal{F}(s) = (s^2 - 1)^2/4$ που παίρνει την ολικά ελάχιστη τιμή 0 στο $s \pm 1$, δηλαδή ικανοποιεί την τιμή $\mathcal{F}(\pm 1) = 0$, βλέπε Εικόνα 1. Η ύπαρξη των δύο σταθερών στάσιμων καταστάσεων του προβλήματος Allen-Cahn συνεπάγεται την μη κυρτή ενέργεια που συνδέεται άμεσα με την εξίσωση. Λόγω της φύσης της μη γραμμικότητας, η λύση u αναπτύσσει χρονικά εξαρτώμενες διεπιφάνειες Γ_t , διαχωρίζοντας περιοχές για τις οποίες $u \approx 1$ από περιοχές όπου $u \approx -1$. Μπορούμε να αναπαραστήσουμε τις προαναφερθείσες διεπιφάνειες ως το σύνολο μηδενικού επιπέδου της συνάρτησης u , $\Gamma_t := \{x \in \Omega : u(x, t) = 0\}$. Ωστόσο, αυτό δεν ορίζει έναν απότομο διαχωρισμό των φάσεων. Πιο συγκεκριμένα, οι φάσεις διαχωρίζονται μέσω μιας περιοχής γύρω από το σύνολο μηδενικού επιπέδου της u , πλάτους ϵ :

$$\Gamma_t \subset Q_t := \{x \in \Omega : |u(x, t)| \leq 1 - \mathcal{O}(\epsilon)\},$$

που ονομάζεται διεπιφάνεια διάχυσης. Εδώ η παράμετρος ϵ ελέγχει το πλάτος της διεπιφάνειας διάχυσης. Η λύση μετακινείται από τη μία περιοχή στην άλλη μέσα στη στενή περιοχή που ονομάζεται διεπιφάνειας διάχυσης. Ένα παράδειγμα που ταιριάζει στο προφίλ των τυπικών λύσεων της εξίσωσης Allen-Cahn δίνεται από

$$u(x) = \tanh \left(d(x)/\sqrt{2}\epsilon \right),$$

όπου $d(x)$ είναι μια προσημασμένη συνάρτηση απόστασης μεταξύ ενός σημείου x στο χωρίο Ω και της διεπιφάνειας Γ_t .



Εικόνα 1: Αριστερά βλέπουμε το διπλό δυναμικό $\mathcal{F}(s) = (s^2 - 1)^2/4$ και στη μέση την παράγωγό του $F(s) = s^3 - s$; οι λύσεις αναπτύσσουν χρονικά εξαρτώμενες διεπιφάνειες Γ_t που διαχωρίσουν τις περιοχές στις οποίες $u(\cdot, t) \approx \pm 1$.

Επιπλέον, η εξίσωση Allen-Cahn αποτελεί την ροή κλίσης του Cahn-Hilliard ενεργειακού συναρτησιακού:

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

που σχετίζεται με το διπλό δυναμικό. Ο πρώτος όρος στο E καλείται ενέργεια όγκου και ο δεύτερος όρος ονομάζεται διεπιφανειακή (δυναμική) ενέργεια. Τότε, η εξίσωση Allen-Cahn προκύπτει ως η L_2 ροή κλίσης

$$u_t = -E'(u), \quad (\text{A.2})$$

$E'(u)$ είναι η Gâteaux παράγωγος στο u .

Μια άλλη ροή κλίσης για το ίδιο ενεργειακό συναρτησιακό (A.1) είναι η εξίσωση Cahn-Hilliard:

$$u_t + \Delta \left(\Delta u - \frac{1}{\epsilon^2} (u^3 - u) \right) = 0, \quad (\text{A.3})$$

όπου πλέον $E'(u)$ είναι η Gâteaux παράγωγος στο u στον χώρο $H^{-1}(\Omega)$. Επιπλέον, το (A.3) αποτελεί διατύπωση του πεδίου φάσης της ροής Hele-Shaw. Εισήχθη αρχικά από τους Cahn-Hilliard για να περιγράψει τα πολύπλοκα φαινόμενα διαχωρισμού φάσεων σε ένα λιωμένο κράμα που αποσβένεται σε τέτοια θερμοκρασία όπου μόνο δύο φάσεις διαφορετικής συγκέντρωσης μπορούν να υπάρχουν ευσταθώς.

Η εξίσωση Allen-Cahn έχει μελετηθεί εκτενώς τις τελευταίες δεκαετίες. Ένα από τα σημαντικότερα θεωρητικά αποτελέσματα είναι η απόδειξη ότι το σύνολο μηδενικού επιπέδου $\Gamma_t^\epsilon := \{x \in \Omega : u(x, t) = 0\}$ εξελίσσεται σύμφωνα με τον γεωμετρικό νόμο της ροής μέσης καμπυλότητας και συγκλίνει στην ακριβή διεπιφάνεια ροής μέσης καμπυλότητας καθώς $\epsilon \rightarrow 0^+$. Η αυστηρή αιτιολόγηση αυτού του ορίου αποτελούσε ένα ανοιχτό πρόβλημα και ολοκληρώθηκε από τους Evans, Soner και Souganidis στο [ESS92].

Καθ' όλη τη διάρκεια της ανάλυσης μελετάμε το πρόβλημα Allen-Cahn, με τις ακόλουθες κατάλληλες αρχικές και συνοριακές συνθήκες:

$$\begin{aligned} u_t - \Delta u + \frac{1}{\epsilon^2} (u^3 - u) &= f && \text{in } \Omega \times (0, T], \\ u &= 0 && \text{στο } \partial\Omega \times (0, T], \\ u(\cdot, 0) &= u_0 && \text{στο } \Omega; \end{aligned} \quad (\text{A.4})$$

υποθέτουμε ότι $\Omega \subset \mathbb{R}^d$ είναι ένα κυρτό, πολυγωνικό ($d = 2$) ή πολυεδρικό ($d = 3$) χωρίο του Ευκλίδειου χώρου \mathbb{R}^d , $T \in \mathbb{R}^+$, $0 < \epsilon \ll 1$, για επαρκώς ομαλή αρχική συνθήκη u_0 και συνάρτηση εξαναγκασμού f .

Η πρόκληση της αριθμητικής επίλυσης του προβλήματος (A.4) προκύπτει από τη μικρή παράμετρο ϵ . Ρεαλιστικά, το ϵ πρέπει να είναι τάξης μεγέθους μικρότερο από το φυσικό πεδίο προσομοίωσης. Επομένως, η ακριβής και αποτελεσματική αριθμητική επίλυση τέτοιων μοντέλων πεδίου φάσης απαιτεί την επίλυση των δυναμικών διεπιφανειών διάχυσης. Οπότε, οι παράμετροι διακριτοποίησης οποιασδήποτε αριθμητικής μεθόδου θα πρέπει να παρέχουν επαρκή αριθμητική εκλέπτυνση για την ακριβή προσέγγιση της εξέλιξης της διεπιφάνειας. Στο πλαίσιο των μεθόδων πεπερασμένων στοιχείων, αυτό συνήθως επιτυγχάνεται μέσω της χρήσης πολύ λεπτών πλεγμάτων στην περιοχή της διεπιφάνειας. Σε μια προσπάθεια προσομοίωσης με προσιτό υπολογιστικό κόστος, ειδικά για $d = 3$, είναι απαραίτητο να αναπτυχθούν προσαρμοστικοί αλγόριθμοι ικανοί να τροποποιούν δυναμικά το μέγεθος του τοπικού πλέγματος.

Όσον αφορά την ανάλυση σφάλματος, μια μεγάλη δυσκολία είναι η εξαγωγή εκτιμήσεων σφάλματος *εκ των προτέρων* και *εκ των υστέρων* που εξαρτώνται από το $1/\epsilon$ μόνο σε χαμηλή πολυωνυμική τάξη. Μια τυπική ανάλυση σφάλματος των προσεγγίσεων με χρήση πεπερασμένων στοιχείων του (A.4) οδηγεί σε εκτιμήσεις *εκ των προτέρων* με δυσμενή εκθετική εξάρτηση από το $1/\epsilon$, κάτι που συμβαίνει αν χρησιμοποιηθεί το τυπικό επιχείρημα ανισότητας τύπου Gronwall. Αυτό έχει περιορισμένη πρακτική αξία ακόμη και για σχετικά μικρό μήκος διεπιφάνειας ϵ . Σύμφωνα με τις εργασίες [Che94, MS95, AF93] ομοιόμορφα φράγματα για την κυρίαρχη ιδιοτιμή του γραμμικοποιημένου χωρικού τελεστή Allen-Cahn γύρω από την αναλυτική λύση u , δηλ.

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

είναι δυνατά εφόσον η εξελισσόμενη διεπιφάνεια Γ_t είναι ομαλή και η $u(t)$ έχει το σωστό προφίλ σε όλη την Γ_t . Τέτοιες φασματικές εκτιμήσεις χρησιμοποιούνται στην εργασία [FP03] για να χειριστούν τον μη γραμμικό όρο στην εξίσωση σφάλματος και αποδεικνύουν *εκ των προτέρων* φράγματα με πολυωνυμική εξάρτηση από το $1/\epsilon$ για μεθόδους πεπερασμένων στοιχείων. Αυτές οι εκτιμήσεις σφαλμάτων επέτρεψαν επίσης την απόδειξη σύγκλισης των αριθμητικών λύσεων στην ακριβή λύση της ροής μέσης καμπυλότητας, καθώς τα μεγέθη διακριτοποίησης του πλέγματος και η παράμετρος ϵ τείνουν στο μηδέν. Επιπλέον, υποθέτοντας μια φασματική εκτίμηση σχετικά με την ακριβή λύση u , έγινε εφικτή η απόδειξη των πρώτων *εκ των υστέρων* εκτιμήσεων σφάλματος στην $L_2(0, T; H^1(\Omega))$ -νόρμα υπό συνθήκη που εξαρτάται μόνο πολυωνυμικά από το ϵ , για μεθόδους πεπερασμένων στοιχείων που προσεγγίζουν το πρόβλημα Allen-Cahn, όπως αυτό παρουσιάστηκε στις εργασίες [KNS04, FW05].

Αυτή η κατεύθυνση της έρευνας έκανε ένα περαιτέρω βήμα με τη θεμελιώδη εργασία [Bar05], όπου η κυρίαρχη ιδιοτιμή του γραμμικοποιημένου χωρικού τελεστή Allen-Cahn για την αριθμητική λύση, U_h ,

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

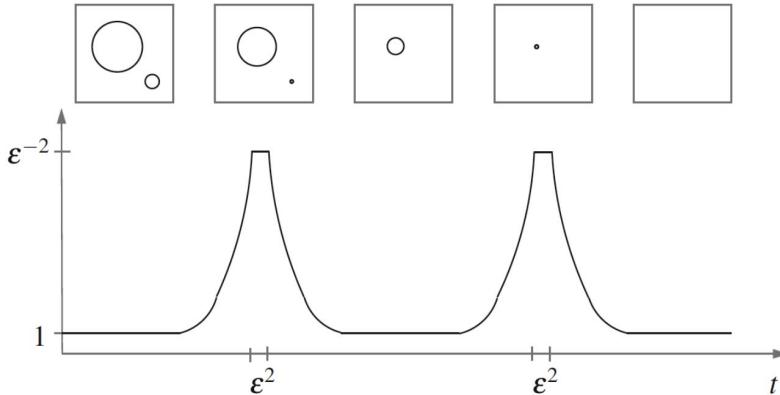
χρησιμοποιείται αντί των *εκ των προτέρων* φράγματων για την $\lambda(t)$ σε μια προσπάθεια να καταλήξει σε πλήρως υπολογίσιμες *εκ των υστέρων* εκτιμήσεις

σφάλματος στις $L_2(0, T; H^1(\Omega))$ - και $L_\infty(0, T; L_2(\Omega))$ -νόρμες. Υπολογίζοντας το $\Lambda(t)$, κάποιος είναι σε θέση να εξάγει σημαντικές πληροφορίες για την ευστάθεια της εξέλιξης από την προσεγγιστική λύση. Η προαναφερθείσα εργασία επικεντρώνεται στην περίπτωση όπου λαμβάνουν χώρα ομαλά εξελισσόμενες διεπιφάνειες.

Όταν η διεπιφάνεια Γ_t υφίσταται τοπολογικές αλλαγές, π.χ. όταν μια διεπιφάνεια καταρρέει, εμφανίζονται μη φραγμένες ταχύτητες και, ως αποτέλεσμα, όλα αυτά τα ομοιόμορφα φράγματα της κυρίαρχης ιδιοτιμής καταρρέουν. Το σημείο κλειδί είναι ότι η κύριαρχη ιδιοτιμή λ μπορεί να κλιψακωθεί όπως $\lambda \sim \epsilon^{-2}$ σε ένα χρονικό διάστημα μήκους συγκρίσιμου με το ϵ^2 . Το **Εικόνα 2** απεικονίζει μια τυπική συμπεριφορά της ιδιοτιμής. Αυτή η κρίσιμη παρατήρηση, που έγινε στο [BMO11], έδειξε ότι η κυρίαρχη ιδιοτιμή μπορεί να θεωρηθεί L_1 -ολοκληρώσιμη ως προς τη μεταβλητή του χρόνου. Τότε, υπάρχει $m > 0$ έτσι ώστε το όριο

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

όπου $x_+ := \max\{x, 0\}$ να ισχύει. Πράγματι, σύμφωνα με το [Bar16, Ενότητα 6.1.4], ο λογαριθμικός όρος προκύπτει από τις περιοχές μετάβασης στις οποίες το λ αυξάνεται όπως $1/(T_c - t)$ για μια τοπολογική αλλαγή που λαμβάνει χώρα την χρονική στιγμή $t = T_c$. Να σημειώσουμε ότι αυτό το όριο είναι αρκετό προκειμένου ώστε να αποφευχθεί η εκθετική εξάρτηση από το αντίστροφο του μήκους της διεπιφάνειας στις εκτιμήσεις που προκύπτουν.



Εικόνα 2: Δύο τοπολογικές αλλαγές σε μια εξέλιξη που ορίζεται από την εξίσωση Allen-Cahn; οι τοπολογικές αλλαγές συνοδεύονται από τις ακραίες κυρίαρχες ιδιοτιμές; Η ιδιοτιμή αυξάνεται όπως $1/(T_c - t)$ πριν συμβεί μια τοπολογική αλλαγή την χρονική στιγμή T_c .

Επιπλέον, οι μετέπειτα εργασίες [BM11, BMO11] εξετάζουν το πιο ρεαλιστικό σενάριο, όταν συμβαίνουν τοπολογικές αλλαγές, και θέτουν την παραπάνω υπόθεση σχετικά με την κυρίαρχη ιδιοτιμή για να εξάγουν αξιόπιστη υπό συνθήκη εκ των υστέρων ανάλυση σφάλματος στις $L_2(0, T; H^1(\Omega))$ - και $L_\infty(0, T; L_2(\Omega))$ -νόρμες. Επιπλέον, οι [BM11], συνδύασαν την ελλειπτική ανακατασκευή που αρχικά προτάθηκε από τους [MN03, LM06] με τεχνικές που αναπτύχθηκαν στο [BMO11] για να εξάγουν σχεδόν βέλτιστες εκ των υστέρων εκτιμήσεις σφάλματος στην $L_\infty(0, T; L_2(\Omega))$ -νόρμα. Αναφερόμαστε επίσης στους [GLV11, CGM13] για την εφαρμογή της ελλειπτικής ανακατασκευής σε μη σύμμιση φρεσκάδας μεθόδους. Ακόμη οι

[GM13] απέδειξαν εκ των υστέρων εκτιμήσεις σφάλματος στις $L_\infty(0, T; L_r(\Omega))$ -νόρμες, $r \in [2, \infty]$, για την ημιδιακριτή περίπτωση της Allen-Cahn.

Στην πρόσφατη εργασία [Chr19], έχουν αποδειχθεί εκ των προτέρων εκτιμήσεις σφάλματος στην $L_4(0, T; L_4(\Omega))$ -νόρμα με σταθερές που φαίνεται να παρέχουν μια μάλλον ευνοϊκή $1/\epsilon$ -πολυωνυμική εξάρτηση. Να σημειωθεί ότι η $L_4(0, T; L_4(\Omega))$ -νόρμα είναι παρούσα στην ευστάθεια του χωρικού τελεστή Allen-Cahn, αν πολλαπλασιάσουμε την (A.4) με u και ολοκληρώσουμε ως προς το χώρο και το χρόνο. Η σημασία της $L_4(0, T; L_4(\Omega))$ -νόρμας φαίνεται κατά την ερμηνεία της εξίσωσης Allen-Cahn ως ροή κλίσης του συναρτησιακού ενέργειας Cahn-Hilliard (A.2). Παρατηρώντας τη διαφορετική κλιμάκωση σε σχέση με το ϵ , είναι προφανές ότι η ποσότητα $(1/\epsilon^2)\|u\|_{L_4(\Omega)}^4$ παίζει καθοριστικό ρόλο. Ένα άμεσο ερώτημα είναι κατά πόσον η απόδειξη υπό συνθήκη εκτιμήσεων σφάλματος στην $L_4(0, T; L_4(\Omega))$ -νόρμα μπορεί επίσης να βελτιώσει την εξάρτηση της συνθήκης από το μήκος διεπιφάνειας ϵ .

Με αφορμή την παραπάνω παρατήρηση, αποδεικνύουμε υπό συνθήκη εκ των υστέρων εκτιμήσεις σφάλματος στην $L_4(0, T; L_4(\Omega))$ -νόρμα για τις πλήρως διακριτές προσεγγίσεις του προβλήματος (A.4). Το αριθμητικό σχήμα περιλαμβάνει την ανάδρομη μέθοδο Euler στο χρόνο σε συνδυασμό με τη μέθοδο πεπερασμένων στοιχείων στο χώρο. Ο χώρος των πεπερασμένων στοιχείων επιτρέπεται να τροποποιείται μεταξύ των χρονικών βημάτων. Η εργασία αυτή, [CGP20], παρουσιάζεται λεπτομερώς στο Κεφάλαιο 3. Το βασικό στοιχείο είναι η εξαγόμενη ϵ -εξάρτηση της συνθήκης που πρέπει ικανοποιείται ώστε να ισχύει η εκτίμησή μας για $d = \{2, 3\}$

$$\eta_d \leq G_d \epsilon^{d+(m-1)/2}, \quad (\text{A.5})$$

για κάποια σταθερά $G_d \geq 1$ και για όλα τα $m \geq 0$. Ως εκ τούτου, η εξάρτηση από το ϵ του εκτιμητή (A.5) φαίνεται να είναι λιγότερο αυστηρή από ότι στο αντίστοιχο αποτέλεσμα στις $L_\infty(0, T; L_2(\Omega))$ - και $L_2(0, T; H^1(\Omega))$ -νόρμες των [Bar05, BM11, BMO11] το οποίο αναφέρει, κατά προσέγγιση, $\tilde{\eta} \leq c\epsilon^{4+3m}$ για τον αντίστοιχο εκτιμητή $\tilde{\eta}$ και κάποια σταθερά $c > 0$. Ως εκ τούτου, η επιδίωξη να αποδείξουμε εκ των υστέρων εκτιμήσεις σφαλμάτων για το $L_4(0, T; L_4(\Omega))$ -νόρμα είναι, κατά την άποψή μας, δικαιολογημένη, καθώς μπορούν δυνητικά να χρησιμοποιηθούν για να για την ανάπτυξη χωροχρονικών προσαρμοστικών αλγορίθμων χωρίς υπερβολικό αριθμό βαθμών ελευθερίας. Είναι καίριας σημασίας ότι τα αποτελέσματα ισχύουν υπό την υπόθεση της ύπαρξης μιας φασματικής εκτίμησης κατά τις τοπολογικές αλλαγές στο πνεύμα του [BMO11].

Η προτεινόμενη ανάλυση βασίζεται σε μια μη συνηθισμένη συνάρτηση δοκιμής η οποία είναι προσεκτικά ορισμένη ώστε να έχει ως αποτέλεσμα τη δημιουργία της νόρμας $\|\cdot\|_{L_4(0,T;L_4(\Omega))}^4$ για τις ποσότητες που απαιτούν εκτίμηση. Ένα βασικό χαρακτηριστικό της νέας συνάρτησης δοκιμής είναι ότι οι ανώτεροι όροι χρονικών και χωρικών σφαλμάτων εμφανίζονται μέσα στις νόρμες $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$. Η απόκλιση των δυνάμεων μεταξύ της νόρμας σφάλματος, $\|\cdot\|_{L_4(0,T;L_4(\Omega))}^4$, και της νόρμας των εκτιμητών, $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$, οδηγεί σε $1/\epsilon$ -εξαρτώμενες σταθερές στους εκτιμητές με τυπικά πιο ήπιες συνθήκες που εξασφαλίζουν την εγκυρότητα των εκ των υστέρων φραγμάτων σφάλματος.

Αποφεύγουμε τις τεχνικές άμεσης προσέγγισης που εκτιμούν τη διαφορά μεταξύ της ακριβούς λύσης και της αριθμητικής προσέγγισης. Συγκεκριμένα, η επιχειρηματολογία συνίσταται στη διάσπαση του ολικού σφάλματος σε δύο μέρη χρησιμοποιώντας μια νέα παραλλαγή της τεχνικής ελλειπτική ανακατασκευή

που παρουσιάζεται στο [GLW21], καθώς και γνωστές ιδέες σχετικά με τη χρονική ανακατασκευή (βλ. [NSV00, MN06, LM06]). Οπότε κάθε όρο του ολικού σφάλματος μπορεί να εκτιμηθεί ξεχωριστά. Μπορούμε να χρησιμοποιήσουμε οποιεσδήποτε διαθέσιμες εκ των υστέρων εκτιμήσεις σφάλματος βασισμένες για ελλειπτικά προβλήματα σε διάφορες νόρμες για να ελέγξουμε το κύριο μέρος του χωρικού σφάλματος, δηλαδή το σφάλμα της ελλειπτικής ανακατασκευής. Είναι γνωστό ότι στο πλαίσιο της μεθόδου πεπερασμένων στοιχείων (ΜΠΣ), η θεωρία των εκ των υστέρων εκτιμήσεων για γραμμικά στάσιμα προβλήματα είναι πολύ ανεπτυγμένη [Ver99, AO00]. Όσον αφορά τον άλλο όρο του ολικού σφάλματος, ικανοποιεί μια παραλλαγή της παραβολικής ΜΔΕ με δεξιά μέλος που μπορούμε να ελέγχουμε με εκ των υστέρων τρόπο. Στη συνέχεια, χρησιμοποιώντας επιχειρήματα ενέργειας και συνέχειας εξάγουμε τις επιθυμητές εκτιμήσεις. Ταυτόχρονα, οι όροι που εμφανίζονται στη δεξιά πλευρά διατηρούν μια τυπική δομή για τα δεδομένα της εκ των υστέρων ανάλυσης: μπορούν να διαχωριστούν ως εκτιμήσεις σφάλματος που σχετίζονται με το χρόνο και το χώρο, ταλαντώσεις δεδομένων και σφάλματα αλλαγής πλέγματος. Ως αποτέλεσμα της μεθόδου απόδειξης, η νέα εκ των υστέρων ανάλυση σφάλματος παρέχει επίσης νέες εκτιμήσεις στις $L_\infty(0, T; L_2(\Omega))$ - και $L_2(0, T; H^1(\Omega))$ -νόρμες που φαίνεται να ισχύουν υπό λιγότερο αυστηρή συνθήκη σε σύγκριση με τα αποτελέσματα της βιβλιογραφίας σε ορισμένες περιπτώσεις.

Η δεύτερη κύρια συμβολή της παρούσας εργασίας είναι η επέκταση του εκ των υστέρων σφάλματος στην περίπτωση μιας χωροχρονικής ασυνεχούς μεθόδου Galerkin αυθαίρετης τάξης επιτρέποντας, ειδικότερα, την διακριτοποίηση του χώρου να αποτελείται από πολύ γενικά πολυγωνικά ($d = 2$) ή πολυεδρικά ($d = 3$) στοιχεία. Συγκεκριμένα, χρησιμοποιούμε την h-p- ασυνεχή μέθοδο Galerkin χρονικού βηματισμού σε συνδυασμό με την ασυνεχή μέθοδο Galerkin εσωτερικής ποινικοποίησης (IPDG) στο χώρο. Αποδεικνύουμε εκ των υστέρων εκτιμήσεις σφάλματος για πλέγματα που αποτελούνται από πολύ γενικά πολυγωνικά και πολυεδρικά στοιχεία σε δύο και τρεις διαστάσεις στο χώρο, αντίστοιχα. Ειδικότερα, αυθαίρετος αριθμός πολύ μικρών επιφανειών επιτρέπεται σε κάθε πολυγωνικό/πολυεδρικό στοιχείο. Η μόνη (πολύ ήπια) προϋπόθεση για το πλέγμα είναι η ύπαρξη μιας υποδιαίρεσης πεπερασμένων μη επικαλυπτόμενων σχηματικά αστεροειδών πολυτοπικών υποστοιχείων, εφόσον ορισμένες υποθέσεις σχηματικής ομαλότητας ανάλογες της [CDG21], ικανοποιούνται. Επιπλέον, παρουσιάζουμε χρήσιμες αντίστροφες εκτιμήσεις και εκτιμήσεις ίχνους που προσαρμόζονται στις ιδιότητες του πλέγματος. Τα παραπόνω αποτελέσματα παρουσιάζονται λεπτομερώς στο Κεφάλαιο 4.

Ο κύριος σκελετός της απόδειξης είναι ανάλογος του Κεφαλαίου 3. Αποφεύγουμε απευθείας τεχνικές για την ανάλυση σφαλμάτων. Διασπάμε το ολικό σφάλμα χρησιμοποιώντας μια ανακατασκευή χώρου-χρόνου, τη λεγόμενη ανακατασκευή χρόνου της ελλειπτικής ανακατασκευής που προτάθηκε από τον [MN03] και μελετήθηκε επιπλέον στις εργασίες [SW10, HW17]. Έτσι, το ολικό σφάλμα αναλύεται σε δύο όρους που μπορούν να περιοριστούν χωριστά. Το κύριο ζητούμενο είναι να φράξουμε από πάνω με πλήρως υπολογίσιμες ποσότητες τον όρο του σφάλματος που είναι συνεχής ως προς την μεταβλητή χρόνου. Για να το κάνουμε αυτό, αναζητούμε μια εξίσωση σφάλματος και στη συνέχεια εφαρμόζουμε κατάλληλα επιχειρήματα ενέργειας και συνέχειας. Για να γίνει αυτό, αναζητούμε μια εξίσωση σφάλματος, η οποία είναι μια τροποποιημένη παραβολική ΜΔΕ, και στη συνέχεια μέσω κατάλληλων επιχειρημάτων ενέργειας και συνέχειας καταλήγουμε σε ένα δεξιά μέρος που αποτελείται από όρους που μπορούν να εκτιμηθούν με εκ των υστέρων τεχνικές. Ο δεύτερος όρος που προκύπτει από τη διάσπαση του

ολικού σφάλματος εκφράζει το σφάλμα της χρονικής ανακατασκευής και το σφάλμα της χωρικής ανακατασκευής και αντιμετωπίζεται με παρόμοιο τρόπο όπως στην [GLW21].

Το σφάλμα ανακατασκευής χώρου πρέπει να αντιμετωπιστεί ως το σφάλμα του ελλειπτικού προβλήματος του οποίου η ασθενής λύση είναι η ελλειπτική ανακατασκευή. Η κύρια δυσκολία που πρέπει να ξεπεράσουμε είναι η έλλειψη της ορθογωνικότητας του σφάλματος ελλειπτικής ανακατασκευής που είναι άμεση συνέπεια της ασυνέπειας της επέκτασης της χωρικής dG-διγραμμικής μορφής σε σχέση με το ελλειπτικό πρόβλημα που δέχεται την ελλειπτική ανακατασκευή ως ασθενή λύση. Για αυτό το λόγο εισάγουμε μια παραλλαγή της έννοιας της ορθογωνικότητας του σφάλματος ελλειπτικής ανακατασκευής στους dG-χώρους. Επιπλέον, αποδεικνύουμε εκτιμήσεις για γραμμικές ασυνεχείς συναρτήσεις κατά στοιχεία με πλήρως υπολογίσιμες σταθερές, τις οποίες χρειαζόμαστε κατά την εφαρμογή επιχειρημάτων δυαδικότητας για να εξαγάγουμε τους εκ των υστέρων ελλειπτικούς εκτιμητές σφάλματος στις $L_p(0, T; L_p(\Omega))$ -νόρμες, $p \geq 2$ για την IPDG μέθοδο σε πολυγωνικά χωρία.

Η τελευταία συνεισφορά αυτής της εργασίας είναι η ανάλυση και η αριθμητική προσέγγιση ενός προβλήματος βέλτιστου ελέγχου που σχετίζεται με το πρόβλημα Allen-Cahn και παρουσιάζεται στα Κεφάλαια 5 και 6, αντίστοιχα. Η εργασία αυτή έχει ήδη υποβληθεί για δημοσίευση [CP22]. Από εδώ και στο εξής, ακολουθούμε τον συνήθη συμβολισμό στα πλαίσια του βέλτιστου ελέγχου: αναφερόμαστε στο y ως τη λύση του προβλήματος Allen-Cahn, ενώ ο εξαναγκαστικός όρος f στο (1.4) αντικαθίσταται από τον έλεγχο που συμβολίζεται με u . Θεωρούμε το ακόλουθο πρόβλημα κατανεμημένου βέλτιστου ελέγχου που εξαρτάται από την εξίσωση Allen-Cahn: ελαχιστοποίησε

$$\begin{aligned} J(u) = & \frac{1}{2} \int_0^T \int_{\Omega} |y_u(t, x) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_{\Omega} |y_u(T, x) - y_{\Omega}(x)|^2 dx \\ & + \frac{\mu}{2} \int_0^T \int_{\Omega} |u(t, x)|^2 dx dt, \end{aligned} \quad (\text{A.6})$$

υπό την προϋπόθεση ότι

$$\begin{aligned} y_{u,t} - \Delta y_u + \frac{1}{\epsilon^2} (y_u^3 - y_u) &= u && \text{in } \Omega_T = \Omega \times (0, T), \\ y_u &= 0 && \text{on } \Sigma_T = \partial\Omega \times (0, T), \\ y_u(\cdot, 0) &= y_0 && \text{in } \Omega. \end{aligned} \quad (\text{A.7})$$

Συγκεκριμένα, στόχος μας είναι να παρέμβουμε στη δυναμική του (A.7) με τη χρήση μιας συνάρτησης ελέγχου u , προκειμένου να εγγυηθούμε ότι η λύση y_u θα είναι όσο το δυνατόν πιο κοντά στον καθορισμένο στόχο y_d . Εδώ $\mu > 0$ είναι ο όρος κανονικοποίησης Tikhonov, ενώ η παρουσία του τερματικού όρου (με $\gamma \geq 0$) είναι απαραίτητη προκειμένου να επιτευχθούν αποτελεσματικές προσεγγίσεις κοντά στο τελικό σημείο του χρονικού διαστήματος. Το σύνολο των αποδεκτών ελέγχων ορίζεται ως:

$$U_{ad} = \left\{ u \in L_2(0, T; L_2(\Omega)) ; u_a \leq u(t, x) \leq u_b \text{ για σ.κ. } (t, x) \in \Omega_T \right\},$$

και το πρόβλημα βέλτιστου ελέγχου στην μειωμένη συναρτησιακή μορφή γραφεται:

$$\begin{cases} \min J(u) \\ u \in U_{ad}. \end{cases} \quad (\text{A.8})$$

Το παραπάνω πρόβλημα βέλτιστου ελέγχου είναι μη κυρτό. Συνεπώς, είναι απαραίτητο να γίνει διάκριση μεταξύ τοπικών και ολικών λύσεων. Ένας έλεγχος $\bar{u} \in U_{ad}$ λέγεται τοπικός βέλτιστος έλεγχος του (A.8) υπό την $L_2(0, T; L_2(\Omega))$ -έννοια, αν υπάρχει $\alpha > 0$ έτσι ώστε $J(\bar{u}) \leq J(u)$ για όλα τα $u \in U_{ad} \cap B_\alpha(\bar{u})$, όπου $B_\alpha(\bar{u})$ είναι η ανοικτή σφαίρα στον $L_2(0, T; L_2(\Omega))$ με κέντρο \bar{u} και ακτίνα α .

Κοινό χαρακτηριστικό στην ανάλυση σφαλμάτος πλήρως διακριτών σχημάτων για προβλήματα βέλτιστου ελέγχου που σχετίζονται με μη γραμμικές παραβολικές ΜΔΕ, υπό περιορισμούς ελέγχου όπως [NV12, CMR19, CC12, CC14, CC16, CC17, HR21] είναι η χρήση αποτελεσμάτων Lipschitz συνέχειας των απεικονίσεων του ελέγχου προς την κατάσταση και της κατάστασης προς την συζυγή κατάσταση, η απόδειξη αναγκαίων και ικανών συνθηκών βελτιστοποίησης πρώτης και δεύτερης τάξης και οι εκτιμήσεις σφαλμάτων των αντίστοιχων απεικονίσεων ελέγχου προς κατάσταση και κατάστασης προς την συζυγή κατάσταση που επιτρέπουν το κλασικό επιχείρημα εντοπισμού [ACT02, CMT05, CR06, CMR07] που αναπτύχθηκε για την ανάλυση σφαλμάτων των σχημάτων διακριτοποίησης για ημιγραμμικά ελλειπτικά προβλήματα ΜΔΕ βελτιστοποίησης με περιορισμούς για να λειτουργεί υπό τις προβλεπόμενες υποθέσεις ομαλότητας.

Ωστόσο, απ' όσο γνωρίζουμε, κανένα από τα παραπάνω αποτελέσματα δεν υπάρχει στην περίπτωση της εξίσωσης Allen-Cahn. Περιλαμβάνει μια μη μονότονη μη γραμμικότητα που ικανοποιεί $\frac{1}{\epsilon^2} F'(s) := \frac{1}{\epsilon^2} (3s^2 - 1) \geq -\frac{1}{\epsilon^2}$. Κατά συνέπεια, για ρεαλιστικές τιμές του ϵ οι κλασικές μέθοδοι απόδειξης συνέχειας Lipschitz της απεικόνισης ελέγχου προς κατάσταση καθώς και η αριθμητική ανάλυση, αποτυγχάνουν αφού εισάγουν σταθερές που εξαρτώνται εκθετικά από το $\frac{1}{\epsilon^2}$. Για την αριθμητική ανάλυση της εξίσωσης Allen-Cahn, όταν $u = 0$, η δυσκολία παρακάμφηκε πρώτη φορά στις θεμελιώδεις εργασίες των [FP03], [KNS04], [FW05], [BMO11], [BM11], όπου απέδειχαν εκτιμήσεις σφαλμάτος (εκ των προτέρων και εκ των υστέρων) για την ομογενή εξίσωση Allen-Cahn με σταθερές που εξαρτώνται πολυωνυμικά από το $\frac{1}{\epsilon}$ με κατάλληλη προσέγγιση της φασματικής εκτίμησης και ένα μη κλασικό επιχείρημα συνέχειας. Δυστυχώς, μια τέτοια ανάλυση απαιτεί συνήθως υποθέσεις ομαλότητας, οι οποίες δεν είναι διαθέσιμες στο πλαίσιο του βέλτιστου ελέγχου. Για παράδειγμα, η υπόθεση $y \in L_\infty(0, T; H^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap H^2(0, T; L_2(\Omega))$ που χρησιμοποιείται στις προαναφερθείσες εργασίες για εκ των προτέρων εκτιμήσεις. Παρόμοιες δυσκολίες προκύπτουν κατά τη ανάλυση και τη αριθμητική ανάλυση της απεικόνισης κατάστασης προς τη συζυγή κατάσταση. Αποδεικνύεται ότι η ανάλυση μπορεί να είναι ακόμη πιο δύσκολη λόγω της απουσίας του κυβικού μη γραμμικού όρου που δημιουργεί τη $L_4(0, T; L_4(\Omega))$ -νόρμα.

Η προσέγγιση της ανάλυσής μας αποφεύγει την κατασκευή οποιασδήποτε διακριτής προσέγγισης μιας φασματικής εκτίμησης και τις υποθέσεις σχετικά με σημειακά χωροχρονικά φράγματα της πλήρως διακριτής λύσης της απεικόνισης του ελέγχου στην κατάσταση. Πράγματι, εφαρμόζουμε τη φασματική εκτίμηση μόνο σε “συνεχές επίπεδο” και όλα τα αποτελέσματά μας ισχύουν για την ομαλότητα που επιβάλλει το πλαίσιο βέλτιστου ελέγχου. Στο Κεφάλαιο 5 μελετάμε τόσο τις απεικονίσεις ελέγχου προς κατάσταση όσο και τις απεικονίσεις κατάστασης προς συζυγούς κατάστασης, προκειμένου να εξάγουμε συνθήκες βελτιστοποίησης πρώτης και δεύτερης τάξης. Το κύριο μέλημα είναι η χρήση τεχνικών που επιτρέπουν την εξαγωγή σταθερών Lipschitz οι οποίες δεν παρουσιάζουν εκθετική εξάρτηση από το $1/\epsilon$. Καταφέρνουμε να αποδείξουμε αποτελέσματα συνέχειας Lipschitz της απεικόνισης ελέγχου σε κατάσταση με σταθερές Lipschitz που είναι ανεξάρτητες από το $1/\epsilon$ εφόσον ισχύει μια υπόθεση εγγύτητας μεταξύ των συναρτήσεων ελέγχου. Όσον αφορά την απεικόνιση της κατάστασης προς την συζυγή κατάσταση,

χρησιμοποιούμε το αποτέλεσμα της συνέχειας Lipschitz της απεικόνισης ελέγχου προς κατάσταση και αποτελέσματα ευστάθειας για να οδηγηθούμε σε σταθερές Lipschitz που εξαρτώνται τουλάχιστον πολυωνυμικά από το $1/\epsilon$.

Η αριθμητική προσέγγιση του προβλήματος βέλτιστου ελέγχου στο κεφάλαιο 6 εξετάζει ένα πλήρως διακριτό σχήμα που συνδυάζει την ασυνεχή μέθοδο Galerkin $dG(0)$ στο χρόνο και τη μέθοδο πεπερασμένων στοιχείων χαμηλότερης τάξης στο χώρο. Ξεκινάμε με την αριθμητική ανάλυση της απεικόνισης ελέγχου προς κατάσταση. Συγκεκριμένα, εξάγουμε *εκ των προστέρων* εκτιμήσεις σφάλματος χρησιμοποιώντας μια προσεκτικά κατασκευασμένη προβολή χώρου-χρόνου, αποτελέσματα διακριτής ευστάθειας και ένα γενικευμένο διακριτό λήμμα Gronwall. Η εξαγωγή των εκτιμήσεων σφάλματος της διακριτής απεικόνισης κατάστασης προς τη συζυγή κατάσταση είναι μια απαιτητική απόδειξη που απαιτεί πολλά τεχνικά ενδιάμεσα στάδια. Συγκεκριμένα, χρειάζεται να αποδείξουμε αποτελέσματα διακριτής ευστάθειας χρησιμοποιώντας ένα δυϊκό και ένα boot-strap επιχείρημα. Τέλος, συνδυάζουμε όλα τα παραπάνω αποτελέσματα για να αποδείξουμε εκτιμήσεις για τη διαφορά μεταξύ των τοπικών βέλτιστων ελέγχων και των διακριτών προσεγγίσεων τους, καθώς και εκτιμήσεις για τις διαφορές μεταξύ της αντίστοιχης κατάστασης και της συζυγούς κατάστασης και των διακριτών προσεγγίσεων τους.

B Κεφάλαιο 3

Το Κεφάλαιο 3 ασχολείται με την απόδειξη *εκ των υστέρων* εκτιμητών σφάλματος για πλήρως διακριτές προσεγγίσεις Galerkin της εξίσωσης Allen-Cahn σε δύο και τρεις χωρικές διαστάσεις. Η αριθμητική μέθοδος περιλαμβάνει την ανάδρομη μέθοδο Euler στον χρόνο σε συνδυασμό με σύμμιορφα πεπερασμένα στοιχεία στο χώρο. Αποδεικνύουμε υπό συνθήκη *εκ των υστέρων* εκτιμήσεις σφαλμάτων στη νόρμα $L_4(0, T; L_4(\Omega))$ που εξαρτώνται πολυωνυμικά από το αντίστροφο του μήκους της διεπιφάνειας ϵ . Εξετάζουμε δύο πιθανά σενάρια όσον αφορά την κίνηση των διεπιφανειών. Συγκεκριμένα, τα αποτελέσματά μας ισχύουν όταν οι εξελισσόμενες διεπιφάνειες είναι ομαλές ακόμη και όταν υφίστανται τοπολογικές αλλαγές. Η απόδειξη βασίζεται στη διάθεση μιας φασματικής εκτίμησης για τον γραμμικοποιημένο τελεστή Allen-Cahn ως προς την προσεγγιστική λύση σε συνδυασμό με ένα επιχείρημα συνέχειας και μια παραλλαγή της ελλειπτικής ανακατασκευής. Η νέα ανάλυση φαίνεται να βελτιώνει τις μέχρι τώρα γνωστές *εκ των υστέρων* εκτιμήσεις σφάλματος στις $L_2(0, T; H^1(\Omega)), L_\infty(0, T; L_2(\Omega))$ -νόρμες σε ορισμένες περιπτώσεις, τουλάχιστον ως προς την ϵ -εξάρτηση της υπό συνθήκη παραδοχής.

B.1 Διακριτοποίηση

Έστω $0 = t_0 < t_1 < \dots < t_N = T$. Χωρίζουμε το δεδομένο χρονικό διάστημα $[0, T]$ σε υποδιαστήματα $J_n := (t_{n-1}, t_n]$ και συμβολίζουμε με $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ κάθε χρονικό βήμα. Έστω επίσης $\{\mathcal{T}_h^n\}_{n=0}^N$ μια ακόλουθια από σύμμιορφες και σχηματικά κανονικές τριγωνοποιήσεις του χωρίου Ω , οι οποίες επιτρέπεται να τροποποιούνται μεταξύ των χρονικών βημάτων. Ορίζουμε τη συνάρτηση μεγέθους πλέγματος, $h_n : \Omega \rightarrow \mathbb{R}$, ως $h_n(x) := \text{diam}(\tau)$, $x \in \tau$ για $\tau \in \mathcal{T}_h^n$. Θα αναφερόμαστε σε $\tau \in \mathcal{T}_h^n$ ως στοιχεία, με τις ακόλουθες ιδιότητες,

$$(i) \quad \bar{\Omega} = \cup_{\tau \in \mathcal{T}_h^n} \bar{\tau},$$

- (ii) για $\tau, \tau' \in \mathcal{T}_h^n$, έχουμε μόνο τις δυνατότητες: είτε $\tau = \tau'$, είτε $\bar{\tau} \cap \bar{\tau}'$ είναι μια κοινή (ολόκληρη) $d - r$ -διάστατη όψη με $1 \leq r < d$ (δηλαδή, όψη, ακμή ή κορυφή, αντίστοιχα).

Σε κάθε τριγωνοποίηση \mathcal{T}_h^n αντιστοιχίζουμε το χώρο πεπερασμένων στοιχείων:

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

με \mathbb{P}_κ να δηλώνει τον χώρο των πολυωνύμων βαθμού το πολύ $\kappa \in \mathbb{N}$.

Λέμε ότι ένα σύνολο τριγωνοποιήσεων είναι συμβατό όταν κατασκευάζονται από διαφορετικές εκλεπτύνσεις της ίδιας τριγωνοποίησης. Έστω δύο συμβατές τριγωνοποιήσεις \mathcal{T}_h^{n-1} και \mathcal{T}_h^n , θεωρούμε το *finest common coarsening* $\hat{\mathcal{T}}_h^n := \mathcal{T}_h^n \wedge \mathcal{T}_h^{n-1}$ και θέτουμε $\hat{h}_n := \max(h_n, h_{n-1})$. Επιπλέον, συμβολίζουμε με \mathcal{S}_h^n τον σκελετό του εσωτερικού πλέγματος της \mathcal{T}_h^n και ορίζουμε τα σύνολα $\hat{\mathcal{S}}_h^n := \mathcal{S}_h^n \cap \mathcal{S}_h^{n-1}$ και $\check{\mathcal{S}}_h^n := \mathcal{S}_h^n \cup \mathcal{S}_h^{n-1}$. Σημειώνουμε ότι καμμία υπόθεση για το σχετικό μέγεθος του \hat{h}_n σε σύγκριση με τα μεγέθη h_{n-1}, h_n δεν είναι απαραίτητη για την εγκυρότητα των εκτιμήσεων που παρουσιάζονται παρακάτω.

Ένας χώρος πεπερασμένων στοιχείων $V_h^n \subset H_0^1(\Omega)$ αντιστοιχεί σε κάθε χρονικό διάστημα $J_n, n = 1, \dots, N$. Στη συνέχεια, αναζητούμε προσεγγιστικές λύσεις στον πλήρως διακριτό χώρο

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

με $\mathbb{P}_0[J_n; V_h^n]$ να δηλώνει το χώρο των σταθερών πολυωνύμων πάνω από J_n , που έχουν τιμές στο V_h^n . Οι συναρτήσεις αυτές επιτρέπεται να είναι ασυνεχείς στα κομβικά σημεία, αλλά θεωρούνται συνεχείς από αριστερά. Παραπέμπουμε στο [Tho06], για περισσότερες λεπτομέρειες σχετικά με τις ασυνεχείς μεθόδους χρονικού βηματισμού Galerkin.

Τώρα είμαστε έτοιμοι να εισαγάγουμε το πλήρως διακριτό σχήμα του (A.4). Για λόγους συντομίας, θέτουμε $F(v) := v^3 - v$. Η ανάδρομη μέθοδος Euler - μέθοδος πεπερασμένων στοιχείων έχει ως εξής: για κάθε $n = 1, \dots, N$, βρείτε $U_h^n \in V_{hk}^n$, έτσι ώστε

$$k_n^{-1} (U_h^n - U_h^{n-1}, X) + (\nabla U_h^n, \nabla X) + \epsilon^{-2} (F(U_h^n), X) = \langle f^n, X \rangle, \quad (B.1)$$

$$U_h^0 = \mathcal{P}_h^0 u^0,$$

για κάθε $X \in V_{hk}^n$. Εδώ, $f^n := f(t_n)$ και \mathcal{P}_h^n η ορθογώνια L_2 -προβολή στον V_h^n , έτσι ώστε $(\mathcal{P}_h^n v, X) = (v, X)$, για όλα τα $X \in V_h^n$. Εισάγουμε τον διακριτό τελεστή Laplace $\Delta_h^n : V_h^n \rightarrow V_h^n$ που ορίζεται από τον τύπο $(-\Delta_h^n V, X) = (\nabla V, \nabla X)$, για όλα τα $V, X \in V_h^n$. Αυτό επιτρέπει την ισχυρή αναπαράσταση του (B.1) ως εξής

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

B.2 Ανακατασκευές

Εισάγουμε μια παραλλαγή της ελλειπτικής ανακατασκευής [MN03, LM06, GLW21], που παίζει καθοριστικό ρόλο στην απόδειξη των εκ των υστέρων εκτιμήσεων σφάλματος.

Ορισμός B.1 (ελλειπτική ανακατασκευή). Για κάθε $n = 0, 1, \dots, N$, ορίζουμε την ελλειπτική ανακατασκευή $\omega^n \in H_0^1(\Omega)$ ως τη λύση του ελλειπτικού προβλήματος

$$(\nabla \omega^n, \nabla v) = \langle g_h^n, v \rangle, \quad \text{για όλα } v \in H_0^1(\Omega), \quad (B.3)$$

όπου

$$\begin{aligned} g_h^n := & -\Delta_h^n U_h^n - \epsilon^{-2} (F(U_h^n) - \mathcal{P}_h^n F(U_h^n)) - \mathcal{P}_h^n f^n + f^n \\ & - k_n^{-1} (\mathcal{P}_h^n U_h^{n-1} - U_h^{n-1}), \end{aligned} \quad (\text{B.4})$$

εδώ και στη συνέχεια υιοθετούμε τη σύμβαση $U_h^{-1} := U_h^0$.

Παρατηρούμε ότι το ω^n ικανοποιεί

$$(\nabla(\omega^n - U_h^n), \nabla X) = 0, \quad \text{για όλα } X \in V_h^n; \quad (\text{B.5})$$

Αυτό συνεπάγεται ότι το $\omega^n - U_h^n$ είναι ορθογώνιο στον V_h^n ως προς το Dirichlet εσωτερικό γινόμενο; μια σημαντική ιδιότητα που μας επιτρέπει να χρησιμοποιήσουμε εκ των υστέρων εκτιμήσεις σφάλματος για ελλειπτικά προβλήματα ώστε να εκτιμήσουμε σε διάφορες νόρμες το σφάλμα του ελλειπτικού προβλήματος (B.3), $\omega^n - U_h^n$, για κάθε $n = 1, \dots, N$ και κάθε $p \geq 2$,

$$\|\omega^n - U_h^n\| \leq \mathcal{E}(U_h^n, g_h^n; L_p(\Omega)). \quad (\text{B.6})$$

Ορίζουμε τις συνεχείς γραμμικές παρεμβολές των ακολουθιών (t_n, U_h^n) και (t_n, ω^n) τις οποίες συμβολίζουμε με $U_h(t)$ και $\omega(t)$ για $t \in (0, T]$:

Ορισμός B.2 (χρονική ανακατασευή). Για $t \in J_n$, $n = 1, \dots, N$, θέτουμε

$$U_h(t) := \ell_{n-1}(t)U_h^{n-1} + \ell_n(t)U_h^n, \quad (\text{B.7})$$

$$\omega(t) := \ell_{n-1}(t)\omega^{n-1} + \ell_n(t)\omega^n, \quad (\text{B.8})$$

όπου ℓ_n η γραμμική συνάρτηση βάσης Lagrange με $\ell_n(t_k) = \delta_{kn}$.

Ο παραπάνω ορισμός συνεπάγεται ότι η χρονική παράγωγος της U_h ,

$$U_{h,t}(t) = (U_h^n - U_h^{n-1})/k_n,$$

είναι η διακριτή διαφορά προς τα πίσω στο t_n .

B.3 Εκ των υστέρων εκτιμήσεις σφάλματος

Θα χρησιμοποιήσουμε τώρα τις ανακατασκευές που ορίστηκαν παραπάνω, μαζί με μη συνήθη επιχειρήματα ενέργειας και συνέχειας και μια φασματική εκτίμηση για το γραμμικοποιημένο τελεστή Allen-Cahn ως προς την προσεγγιστική λύση U_h , για να καταληξουμε σε εκ των υστέρων εκτιμήσεις σφάλματος στις $L_4(0, T; L_4(\Omega))$ -, $L_2(0, T; H^1(\Omega))$ - και $L_\infty(0, T; L_2(\Omega))$ -νόρμες. Ξεκινάμε με τη διάσπαση του ολικού σφάλματος ως εξής:

$$e := u - U_h = \theta - \rho, \quad \text{όπου } \theta := \omega - U_h, \rho := \omega - u.$$

Αρχικά, η διαφορά θ μπορεί να εκτιμηθεί μέσω εκ των υστέρων εκτιμήσεων σφάλματος για ελλειπτικά προβλήματα σε διάφορες νόρμες εφαρμόζοντας κατάλληλα δυϊκά επιχειρήματα. Επίσης, η διαφορά ρ ικανοποιεί μια παραβολικού τύπου εξίσωση με πλήρως υπολογίσιμο δεξί μέλος που αποτελείται από τον όρο θ και τα δεδομένα του προβλήματος. Το ακόλουθο Λήμμα δηλώνει αυτή την εξίσωση σφάλματος.

Λήμμα B.3 (εξίσωση σφάλματος). Στο J_n , $n = 1, \dots, N$ και για όλα τα $v \in H_0^1(\Omega)$, έχουμε

$$\begin{aligned} & \langle \rho_t, v \rangle + (\nabla \rho, \nabla v) + \epsilon^{-2} (F(U_h) - F(u), v) \\ &= \langle f^n - f, v \rangle + \langle \theta_t, v \rangle + \epsilon^{-2} (F(U_h) - F(U_h^n), v) + (\nabla(\omega - \omega^n), \nabla v). \end{aligned} \quad (\text{B.9})$$

Στο σημείο αυτό εισάγουμε ορισμένους συμβολισμούς που θα χρειαστούμε στη συνέχεια για την παρουσίαση των βασικών αποτελεσμάτων που αφορούν τις εκ των υστέρων εκτιμήσεις του ρ . Θέτουμε σε κάθε J_n , $n = 1, \dots, N$ τα ακόλουθα:

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

Ο όρος \mathcal{L}_1 και ο όρος $\epsilon^{-4} \| F(U_h) - F(U_h^n) \|_{L_2(\Omega)}^2$ του \mathcal{L}_2 αποκαλούνται συχνά χρονικές εκτιμήσεις σφάλματων στη βιβλιογραφία ενώ $\| f^n - f \|_{L_2(\Omega)}^2$ είναι η προσέγγιση δεδομένων. Επίσης, $C_0 := (\tilde{c}^2 + 1)/2$, $C_1 := 9 + 9C_P\tilde{c}^2 + 6^4 11^2 C_P^2 \tilde{c}^4$ και $C_2 := 2 \cdot 3^7 C_P^2 \tilde{c}^4$, C_P όπως στην (2.8) ενώ \tilde{c} όπως στις (2.3)-(2.5), έτσι ώστε

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

Θ_1 αντιπροσωπεύει την μεταβολή του πλέγματος και το Θ_2 (ή $\tilde{\Theta}_2$ για $d = 3$) συχνά αποκαλείται εκτίμηση του χωρικού σφάλματος. Πράγματι, αποδεικνύουμε για $p \geq 2$

$$\begin{aligned} & \| \theta \|_{L_p(\Omega)} \leq \mathcal{E}(U_h^n, g_h^n; L_p(\Omega)) + \mathcal{E}(U_h^{n-1}, g_h^{n-1}; L_p(\Omega)) \\ & \mathcal{E}(U_h^n, g_h^n; L_p(\Omega)) := C_\Omega C_{SZ} \left(\sum_{\tau \in \mathcal{T}_h^n} \| h_n^2 r_n \|_{L_p(\tau)}^p + \sum_{e \in \mathcal{S}_h^n} \| h_n^{1+1/p} [\nabla U_h^n] \|_{L_p(e)}^p \right)^{1/p}, \\ & \text{ενώ } \gamma p = \infty \\ & \mathcal{E}(U_h^n, g_h^n; L_\infty(\Omega)) := C \ell_{h,d} \left(\sum_{\tau \in \mathcal{T}_h^n} \| h_n^2 r_n \|_{L_\infty(\tau)} + \sum_{e \in \mathcal{S}_h^n} \| h_n [\nabla U_h^n] \|_{L_\infty(e)} \right); \end{aligned}$$

$\ell_{h,d} = (\ln(1/h_n))^{\alpha_d}$, όπου $\alpha_2 = 2$ και $\alpha_3 = 1$; βλ. [DG12, Theorem 6.1]. Εδώ, $[\nabla U_h^n]$ είναι το άλμα κατά μήκος του e και $r_n := g_h^n + \Delta U_h^n$ το υπόλοιπο ανά στοιχείο του ελλειπτικού προβλήματος (B.3) την χρονική στιγμή t_n που αποτελεί ταυτόχρονα και το υπόλοιπο του προτεινόμενου αριθμητικού σχήματος (B.1). Τέλος, αποδεικνύουμε εκ των υστέρων εκτιμητές για $p = 2, 4, 6$ της μορφής:

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

όπου

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

Ένα βασικό βήμα στην απόδειξη του ακόλουθου λήμματος για $d = 2$ και 3 είναι η επιλογή μιας μη συνηθισμένης συνάρτησης ελέγχου $v = \phi$ (3.17) για την εξίσωση σφάλματος (B.9). Αυτή η συνάρτηση δοκιμής είναι υπεύθυνη για την εμφάνιση του όρου $\|\rho\|_{L_4(0,T;L_4(\Omega))}^4$, μαζί με άλλους μη αρνητικούς όρους στην αριστερή πλευρά του (B.10) κατά τη διάρκεια του ενεργειακού επιχειρήματος. Ταυτόχρονα, αυτή η συνάρτηση δοκιμής είναι επίσης υπεύθυνη για την παρουσία ευνοϊκών υπολογίσμων όρων σφάλματος στη νόρμα $\|\cdot\|_{L_2(0,T;L_2(\Omega))}^2$, βλ. τους όρους στο $\int_0^\tau (\mathcal{L}_1 + \mathcal{L}_2) dt$ που τελικά θα εμφανιστούν στην τελική εκτίμηση. Έτσι, η εξάρτηση από το ϵ των σταθερών που πολλαπλασιάζουν διάφορους όρους των \mathcal{L}_1 και \mathcal{L}_2 θα μειωθεί στο μισό λόγω της ασυμφωνίας μεταξύ της $4^{\text{ης}}$ δύναμης που εμφανίζεται στους όρους σφάλματος και της $2^{\text{ης}}$ δύναμης στους αντίστοιχους εκτυπητές. Αυτή η παρατήρηση οδηγεί σε μια τυπικά καλύτερη εξάρτηση ως προς το $1/\epsilon$ στο επιχείρημα της συνέχειας. Ταυτόχρονα, η επιλογή (3.17) οδηγεί σε όρους που περιέχουν $\|\theta\|_{L_4(0,T;L_4(\Omega))}^4$, $\|\theta\|_{L_6(0,T;L_6(\Omega))}^6$, και $\|\theta_t\|_{L_4(0,T;L_4(\Omega))}^4$ χωρίς να επιβαρύνεται η τυπική εξάρτηση από το ϵ^{-1} , όπως θα δούμε στη συζήτηση παρακάτω. Οι τελευταίοι όροι είναι ‘συμβατοί’ με τις νόρμες του σφάλματος ρ που εμφανίζονται στο (B.10).

Λήμμα B.4 ($d = 2$). Έστω $d = 2$ και u η λύση της (3.1) και ω όπως στην (B.8). Υποθέτουμε ότι $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ για σ.κ. $t \in (0, T]$. Τότε, για κάθε $\tau \in (0, T]$, έχουμε

$$\begin{aligned} & \frac{1}{4} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ & + \int_0^\tau A(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2} \right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h) \rho, \rho) \right) dt \\ & \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \Theta_2 + C_0(\mathcal{L}_1 + \mathcal{L}_2)) dt \quad (\text{B.10}) \\ & + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \alpha(U_h) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ & + \frac{1}{4\epsilon^6} \int_0^\tau \left(\beta(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \gamma(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt, \end{aligned}$$

όπου

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

Λήμμα B.5 ($d = 3$). Έστω $d = 3$ και u η λύση της (3.1) και ω όπως στην (B.8). Υποθέτουμε ότι $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ για σ.κ. $t \in (0, T]$. Τότε, για κάθε $\tau \in (0, T]$,

έχουμε

$$\begin{aligned}
& \frac{1}{8} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\
& + \int_0^\tau A(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U_h) \rho, \rho) \right) dt \\
& \leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1 + \tilde{\Theta}_2 + \tilde{C}_0 (\mathcal{L}_1 + \mathcal{L}_2)) dt \quad (\text{B.11}) \\
& + \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + (\alpha(U_h) + 1) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\
& + \frac{1}{4\epsilon^{10}} \int_0^\tau \left(\tilde{\beta}(\theta, U_h) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \tilde{\gamma}(\theta, U_h) \|\rho\|_{L_2(\Omega)}^4 \right) dt,
\end{aligned}$$

όπου συμβολίζουμε με

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

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

Αν ισχύει οποιαδήποτε περίπτωση της παραδοχής 3.11, έχουμε ότι

$$\begin{aligned}
& \|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U_h) \rho, \rho) \\
& \geq -\bar{\Lambda}(t) (1 - \epsilon^2) \|\rho\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U_h) \rho, \rho). \quad (\text{B.12})
\end{aligned}$$

Εισάγουμε την (B.12) στις (B.10) και (B.11) όταν $d=2$ και 3, αντίστοιχα, και εφαρμόζουμε ένα επιχείρημα συνέχειας αντίστοιχο του Λήμματος 2.5. Θέτουμε τις ποσότητες:

$$\begin{aligned}
\mathcal{N}_{[0,\tau],d}(\rho) &:= \frac{1}{4(d-1)} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{\epsilon^2}{2} \int_0^\tau \|\nabla \rho\|_{L_2(\Omega)}^2 dt \\
&+ \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \sup_{t \in [0,\tau]} \frac{1}{2} \|\rho\|_{L_2(\Omega)}^2, \quad d = 2, 3. \\
\eta_2 &:= \left(\frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \sum_{n=1}^N \int_{J_n} (\Theta_1 + \Theta_2 + C_0 (\mathcal{L}_1 + \mathcal{L}_2)) dt \right)^{1/4}, \\
\mathcal{D}_2 &:= \max\{4, \alpha(U_h) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 2\}, \mathcal{B}_2 := \max\{16\beta(\theta, U_h), \gamma(\theta, U_h)\}, \\
\bar{\mathcal{B}}_2 &:= \sup_{t \in [0,T]} \mathcal{B}_2(t), E_2 := \exp\left(\int_0^T \mathcal{D}_2(t) dt\right), \\
\eta_3 &:= \left(\frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \sum_{n=1}^N \int_{J_n} (\Theta_1 + \tilde{\Theta}_2 + \tilde{C}_0 (\mathcal{L}_1 + \mathcal{L}_2)) dt \right)^{1/4}, \\
\mathcal{D}_3 &:= \max\{4, \alpha(U_h) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 3\}, \mathcal{B}_3 := \max\{16\tilde{\beta}(\theta, U_h), \tilde{\gamma}(\theta, U_h)\}, \text{ και} \\
\bar{\mathcal{B}}_3 &:= \sup_{t \in [0,T]} \mathcal{B}_3(t), E_3 := \exp\left(\int_0^T \mathcal{D}_3(t) dt\right), \text{ και καταλήγουμε στην ακόλουθη} \\
&\text{υπο συνθήκη εκτίμηση για την ποσότητα } \rho:
\end{aligned}$$

Λήμμα B.6. Υποθέτουμε ότι ισχύει

$$\eta_2^4 \leq \epsilon^6 (16\bar{\mathcal{B}}_2(T+1)E_2^2)^{-1}, \quad \text{όταν } d=2, \quad (\text{B.13})$$

$$\eta_3^4 \leq \epsilon^{10} (16\bar{\mathcal{B}}_3(T+1)E_3^2)^{-1}, \quad \text{όταν } d=3. \quad (\text{B.14})$$

Τότε, έχουμε την εκτίμηση για

$$\mathcal{N}_{[0,T],d}(\rho) \leq 4\eta_d^4 E_d, \quad \text{όταν } d=2,3. \quad (\text{B.15})$$

Τώρα είμαστε έτοιμοι να παρουσιάσουμε την κύρια εκτίμηση σφάλματος στην $L_4(0,T;L_4(\Omega))$ -νόρμα.

Θεώρημα B.7. Έστω $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ και $f \in L_\infty(0,T;L_4(\Omega))$, $\Omega \subset \mathbb{R}^d$, $d=2,3$. Έστω u η λύση της (3.1) και U_h η προσέγγιση της (B.1). Τότε, σύμφωνα με την υπόθεση (3.11)(II) και τη συνθήκη

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

ισχύει η ακόλουθη εκτίμηση

$$\|u - U_h\|_{L_4(0,T;L_4(\Omega))} \leq 2\eta_d ((d-1)E_d)^{1/4} + \|\theta\|_{L_4(0,T;L_4(\Omega))}. \quad (\text{B.17})$$

Τονίζουμε ότι το Θεώρημα ισχύει επίσης σε περιπτώσεις όπου δεν είναι δυνατό να υποθέσουμε ότι η $\|U_h\|_{L_\infty(0,T;L_\infty(\Omega))}$ φράσσεται ανεξάρτητα από το $1/\epsilon$. Σημειώνουμε, ωστόσο, ότι η $\|U_h\|_{L_\infty(0,T;L_\infty(\Omega))}$ παραμένει ομοιόμορφα φραγμένη ως προς το $1/\epsilon$ και τις παραμέτρους του πλέγματος σε όλα τα σενάρια πρακτικού ενδιαφέροντος που γνωρίζουμε και συνήθως απαιτείται σε σενάρια που εξασφαλίζουν την εγκυρότητα της παραδοχής 3.11.

Είναι διδακτικό να συζητήσουμε λεπτομερώς την εξάρτηση των διαφόρων όρων που εμφανίζονται στις (B.16) και (B.17) για να αξιολογήσουμε την πρακτικότητα του παραγόμενου εκ των υστέρων φράγματος του σφάλματος. Η υπολογιστική πρόκληση για το $\epsilon \ll 1$ εκδηλώνεται με την ικανοποίηση της συνθήκης (B.16). Πράγματι, καθώς $\epsilon \rightarrow 0$ η συνθήκη (B.16) γίνεται όλο και πιο αυστηρή για να ικανοποιηθεί, απαιτώντας τα πλέγματα να είναι τοπικά όλο και πιο λεπτά ώστε να μειωθεί ο εκτιμητής η_d - αυτό έχει ως αποτέλεσμα την αύξηση των βαθμών ελευθερίας. Μόλις το η_d είναι αρκετά μικρό, ένας προσαρμοστικός αλγόριθμος θα μπορούσε να χρησιμοποιήσει το θεώρημα για περαιτέρω εκτίμηση.

Ας υποθέσουμε για λόγους επιχειρηματολογίας ότι $\|U_h^n\|_{L_\infty(\Omega)} \leq C'$ για όλα τα $n = 1, \dots, N$ για κάποια ανεξάρτητη από το ϵ σταθερά $C' > 0$. Επίσης, έχουμε

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

Προς το παρόν, αν υποθέσουμε ότι $\|\theta^n\|_{L_\infty(\Omega)} \leq C'$ ομοιόμορφα ως προς το ϵ , τότε μπορούμε να συμπεράνουμε ότι $2^4 \cdot 6 \leq \bar{\mathcal{B}}_d \leq CC'$, $d=2,3$ και, επομένως,

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

για κάποιες γενικές σταθερές $C > 0$, ανεξάρτητες από το ϵ , αφού σημειωθεί ότι $\sqrt[4]{6} > 1.5$. Επιπλέον, στην περίπτωση ομαλά αναπτυσσόμενων διεπιφανειών (Υπόθεση 3.11(I)), αναμένεται ότι $E_d \sim 1$, σύμφωνα με τις κλασικές εργασίες [Che94, MS95]. Όταν λαμβάνουν χώρα τοπολογικές αλλαγές, μπορούμε ανάλογα με την

[BMO11] να θεωρήσουμε ότι $E_d \sim \epsilon^{-m}$, $m > 0$. Με την παραπάνω σύμβαση, η (B.16) γίνεται

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

για κάποια σταθερά $G_d \geq 1$ και για όλα τα $m \geq 0$, περικλείοντας έτσι ταυτόχρονα και τις δύο περιπτώσεις της Υπόθεσης 3.11.

Ως εκ τούτου, η ϵ -εξάρτηση της συνθήκης (B.16) φαίνεται να είναι λιγότερο περιοριστική από ό,τι στην αντίστοιχη εκ των υστέρων ανάλυση στις $L_\infty(0, T; L_2(\Omega))$ -και $L_2(0, T, H^1(\Omega))$ -νόρμες των [Bar05, BMO11, BM11], όπου $\tilde{\eta} \leq c\epsilon^{4+3m}$ για τον αντίστοιχο εκτιμητή $\tilde{\eta}$ και κάποια σταθερά $c > 0$. Η νέα εκ των υστέρων ανάλυση σφάλματος φαίνεται να βελτιώνει επίσης την ϵ -εξάρτηση από τη συνθήκη για $L_2(0, T; H^1(\Omega))$ - και $L_\infty(0, T, L_2(\Omega))$ -νόρμες σε σύγκριση με [FW05, Bar05, BMO11, BM11] σε ορισμένες περιπτώσεις. Συγκεκριμένα, έχουμε το ακόλουθο αποτέλεσμα.

Πρόταση B.8 ($L_2(H^1)$ -και $L_\infty(L_2)$ -εκτιμήσεις). Με τις υποθέσεις του Θεωρήματος B.7 και υποθέτοντας τη συνθήκη (B.16), έχουμε ότι

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

Επομένως, στο ίδιο πλαίσιο με πριν, έχουμε ότι (B.16) συνεπάγεται

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

Αν δεχτούμε ότι $\eta_d^2 \sim \tilde{\eta}$ από το [Bar05, BMO11, BM11], για χάρη του επιχειρήματος, τουλάχιστον στο επίπεδο της υπό συνθήκη εκτίμησης, (3.37) δίνει τυπικά ευνοϊκή εξάρτηση από το ϵ όταν $d = 2$ και $m \geq 0$ και επίσης όταν $d = 3$ και $m \geq 1/2$, σε σύγκριση με την αντίστοιχη εξάρτηση $\tilde{\eta} \leq c\epsilon^{4+3m}$ στις προηγούμενες εργασίες [BMO11, BM11].

C Κεφάλαιο 4

Στο Κεφάλαιο 4 εστιάζουμε στην απόδειξη εκ των υστέρων εκτιμήσεων σφάλματος για τις πλήρως διακριτές προσεγγίσεις της εξίσωσης Allen-Cahn (1.4) σε δύο και τρεις χωρικές διαστάσεις, για την αριθμητική μέθοδο που συνδυάζει τη μέθοδο ασυνεχούς χρονικού βηματισμού Galerkin (DG) με την ασυνεχή μέθοδο Galerkin εσωτερικής ποινικοποίησης (IPDG) στο χώρο. Όσον αφορά το χωρίο διασπάται σε γενικά πολύτοπα, ενώ επιτρέπεται αυθαίρετος αριθμός πολύ μικρών όψεων. Το βασικό κίνητρο για τη μελέτη αυτής της μεθόδου είναι οι δυνατότητες που προσφέρει για σημαντική μείωση της υπολογιστικής πολυπλοκότητας με τη χρήση “μεγάλων” στοιχείων γενικού σχήματος σε περιοχές της λύσης, $u \approx \pm 1$, ενώ χρησιμοποιούνται εξαιρετικά εκλεπτυσμένα στοιχεία στις περιοχές της διεπιφάνειας για την επίλυση των στρωμάτων. Η ομαλότητα του πλέγματος είναι ανάλογη της [CDG21]. Για τη μέθοδο αυτή, αποδεικνύουμε εκ των υστέρων εκτιμήσεις σφαλμάτων στις νόρμες $L_4(0, T; L_4(\Omega))$, $L_2(0, T; H^1(S))$ και $L_\infty(0, T; L_2(\Omega))$ που εξαρτώνται πολυωνυμικά από το αντίστροφο του μήκους της διεπιφάνειας ϵ , υπό συνθήκες. Οι συνθήκες παρουσιάζουν ανάλογη εξάρτηση από το ϵ με το απλούστερο πλήρως διακριτό σχήμα του Κεφαλαίου 3. Αυτή τη φορά, εισάγουμε την

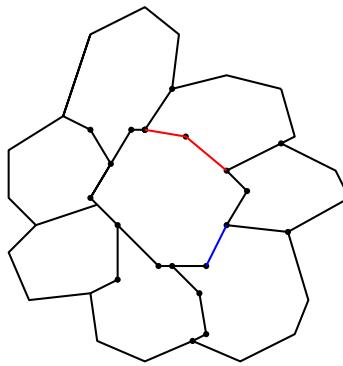
ιδέα της ανακατασκευής χώρου-χρόνου για την διάσπαση του ολικού σφάλματος, που προκύπτει από το συνδυασμό της ανακατασκευής χρόνου όπως εισήχθη στο [MN06] και μελετήθηκε περαιτέρω στις [SW10, HW17, GLW21] και μιας παραλλαγής της ελλειπτικής ανακατασκευής [MN03, LM06] που λαμβάνει υπόψη το φαινόμενο της αλλαγής πλέγματος. Ανάλογα με το προηγούμενο κεφάλαιο, εφαρμόζουμε μη κλασικές ενεργειακές τεχνικές μαζί με ένα επιχείρημα συνέχειας για να εξάγουμε έναν εκτιμητή με όρους που μπορούν να εκτιμηθούν με εκ των υστέρων τεχνικές. Πάλι είναι κρίσιμης σημασίας η φασματική εκτίμηση του γραμμικοποιημένου τελεστή Allen-Cahn σε σχέση με την προσεγγιστική λύση του προτεινόμενου σχήματος. Η διατύπωση της εκ των υστέρων εκτίμησης σφάλματος απαιτεί ένα κάτω φράγμα της κύριαρχης ιδιοτιμής; για το σκοπό αυτό υιοθετούμε την υπόθεση 3.11. Επιπλέον, μελετάμε την προσέγγιση του προβλήματος ιδιοτιμών με μια μέθοδο hp -πεπερασμένων στοιχείων και εξάγουμε αντίστοιχες εκτιμήσεις σφάλματος.

C.1 Διακριτοποίηση

Έστω $0 = t_0 < t_1 < \dots < t_N = T$. Θεωρούμε την διαμέριση του χρονικού διαστήματος $[0, T]$ σε υποδιαστήματα $J_n := (t_{n-1}, t_n]$ όπου $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ το χρονικό βήμα. Έστω επίσης $\{\mathcal{T}_h^n\}_{n=0}^N$ μια ακολουθία υποδιαιρέσεων του χωρίου Ω σε γενικά πολυγωνικά ($d=2$) ή πολυεδρικά ($d=3$) στοιχεία τ , τα οποία επιτρέπεται να τροποποιούνται σε κάθε χρονικό βήμα. Συμβολίζουμε με $h_\tau := \text{diam}(\tau)$ τη διάμετρο του $\tau \in \mathcal{T}_h^n$. Αντιστοιχίζουμε σε κάθε \mathcal{T}_h^n τον ασυνεχή ανά στοιχείο πολυωνυμικό χώρο:

$$S_h^n := \{v_h \in L_2(\Omega); v_h|_\tau \in \mathbb{P}_\kappa(\tau), \forall \tau \in \mathcal{T}_h^n\},$$

με \mathbb{P}_κ να δηλώνει τον d -μεταβλητό χώρο των πολυωνύμων βαθμού το πολύ $\kappa \in \mathbb{N}$. Έστω $\Gamma^n := \cup_{\tau \in \mathcal{T}_h^n} \partial\tau$ ο σκελετός του πλέγματος, ενώ $\Gamma_{\text{int}}^n := \Gamma^n \setminus \partial\Omega$ το εσωτερικό του έτσι ώστε $\Gamma^n = \partial\Omega \cup \Gamma_{\text{int}}^n$. Ο σκελετός αναλύεται σε $(d-1)$ -διάστατες όψεις, που μοιράζονται το πολύ δύο στοιχεία. Διαφέρουν από τις διεπιφάνειες, που ορίζονται ως οι απλά συνεκτικές συνιστώσες της τομής δύο γειτονικών στοιχείων. Οι hanging κόμβοι/ακμές επιτρέπονται καθώς μια διεπιφάνεια μπορεί να είναι πολυσχιδής. Δείτε την Εικόνα 3 για μια απεικόνιση για $d=2$.



Εικόνα 3: Πολυγωνικό στοιχείο $\tau \in \mathcal{T}_h^n$, και οι γειτονές του ανά πλευρά; οι hanging κόμβοι σημειώνονται με έντονες κουκκίδες.

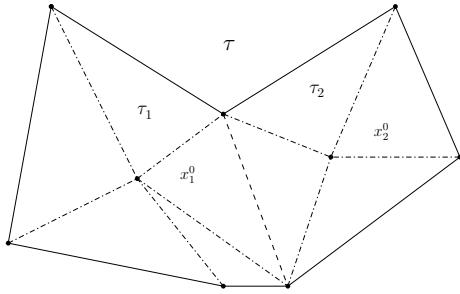
Υιοθετούμε τις υποθέσεις ομαλότητας του πλέγματος στην φιλοσοφία των [CDG21] με μικρές τροποποιήσεις. Συγκεκριμένα, για κάθε $n = 1, \dots, N$ έχουμε:

Υπόθεση C.1 (Ομαλότητα πλέγματος, [CDG21]). Κάθε στοιχείο $\tau \in \mathcal{T}_h^n$ είναι μια πεπερασμένη ένωση σχηματικά αστεροειδών πολυτόπων. Υπάρχει μια υποδιαίρεση κάθε τ από πεπερασμένα μη επικαλυπτόμενα πολύτοπα $\{\tau_i\}_{i=1}^{n_\tau}$, τα οποία είναι σχηματικά αστεροειδή ως προς ένα σημείο $\mathbf{x}_i^* \in \tau_i$ έτσι ώστε

$$C_{\text{sh}} \mathbf{m}_i(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \geq h_\tau,$$

όπου $\mathbf{m}_i(\mathbf{x}) := \mathbf{x} - \mathbf{x}_i^*$, $\mathbf{x} \in \partial\tau_i$ και $\mathbf{n}(\mathbf{x})$ το μοναδιαίο κανονικό διάνυσμα στο $\mathbf{x} \in \partial\tau_i$. Εδώ, $C_{\text{sh}} > 1$ είναι μια σταθερά ανεξάρτητη του h_τ που ισχύει ομοιόμορφα σε όλες τις αλλαγές πλέγματος κατά τη διάρκεια των χρονικών βημάτων. Επιπλέον, υπάρχει $n_e \in \mathbb{N}$ τέτοια ώστε για κάθε $\tau \in \mathcal{T}_h^n$ και κάθε απλά συνεκτική διεπιφάνεια $I \subset \Gamma^n \cap \partial\tau$,

$$\text{αν } C_{\text{sh}} |I| \leq h_\tau^{d-1}, \text{ τότε } \text{card}\{e \in \Gamma^n : e \subset I\} \leq n_e.$$



Εικόνα 4: πολυγωνικό στοιχείο $\tau \in \mathcal{T}_h^n$ με εφτά κόμβους; χωρίζεται σε δύο σχηματικά αστεροειδή πολύγωνα τ_1, τ_2 ως προς τα x_1^0 και x_2^0 , αντίστοιχα.

Δοθέντων τ^+, τ^- που μοιράζονται μια $(d-1)$ -διάστατη όψη $e := \tau^+ \cap \tau^- \subset \Gamma_{\text{int}}^n$ με \mathbf{n}^+ και \mathbf{n}^- τα αντίστοιχα κανονικά μοναδιαία διανύσματα στο e με κατεύθυνση προς τα έξω. Ορίζουμε μέσους όρους και άλματα σε κάθε e , $v : \Omega \rightarrow \mathbb{R}$, $\mathbf{w} : \Omega \rightarrow \mathbb{R}^d$ ως έξής:

$$\begin{aligned} \{v\}|_e &:= \frac{1}{2} (v^+ + v^-), \quad \{\mathbf{w}\}|_e := \frac{1}{2} (\mathbf{w}^+ + \mathbf{w}^-), \\ \llbracket v \rrbracket|_e &:= v^+ \mathbf{n}^+ + v^- \mathbf{n}^-, \quad \llbracket \mathbf{w} \rrbracket|_e := \mathbf{w}^+ \cdot \mathbf{n}^+ + \mathbf{w}^- \cdot \mathbf{n}^-. \end{aligned}$$

$$v^\pm := v|_{e \cap \partial\tau^\pm}, \mathbf{w}^\pm := \mathbf{w}|_{e \cap \partial\tau^\pm}. \text{ Αν } e \subset \partial\tau \cap \partial\Omega, \text{ θέτουμε } \{\mathbf{w}\} := \mathbf{w}^+, \llbracket v \rrbracket := v^+ \mathbf{n}^+.$$

Ένας χώρος πεπερασμένων στοιχείων S_h^n ορίζεται σε κάθε χρονικό διάστημα J_n , $n = 1, \dots, N$. Αναζητούμε προσεγγιστικές λύσεις από το χώρο

$$S_{hk} := \left\{ V : (0, T] \rightarrow L_2(\Omega); V|_{J_n} \in \mathbb{P}_{q_n}(J_n; S_h^n) \text{ για κάθε } n = 1, \dots, N \right\},$$

$\mathbb{P}_{q_n}(J_n; S_h^n)$ δηλώνει το χώρο των πολυωνύμων βαθμού το πολύ $q_n \in \mathbb{N}_0$, με τιμές στο S_h^n . Οι συναρτήσεις αυτές είναι αριστερά συνεχείς με δεξιά όρια και γράφουμε X_n^+ για $X(t_n) = X(t_n^-)$ και X_n^+ για $X(t_n^+)$. Το άλμα στον χρονικό κόμβο t_n συμβολίζεται $\llbracket X \rrbracket_n = X_n^+ - X_n^-$. Τα παραπάνω προτείνουν την ακόλουθη χωροχρονική ασυνεχή μέθοδο Galerkin του (1.4): Βρείτε $U \in S_{hk}$ τέτοια ώστε

$$U(0) = U(t_0^-) := P_h^0 u_0, \tag{C.1}$$

και για $n = 1, \dots, N$ και για κάθε $V \in \mathbb{P}_{q_n}(J_n; S_h^n)$,

$$\begin{aligned} & \int_{J_n} ((U_t, V) + B_n(U, V)) dt + ([U]_{n-1}, V_{n-1}^+) + \epsilon^{-2} \int_{J_n} (F(U), V) dt \\ &= \int_{J_n} (f, V) dt, \end{aligned} \quad (\text{C.2})$$

$B_n := B_n(t) = S_h^n \times S_h^n \rightarrow \mathbb{R}$ είναι η χωρική ασυνεχή Galerkin διγραμμική μορφή που δίνεται από τη σχέση

$$\begin{aligned} B_n(w, v) &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla w \cdot \nabla v dx \\ &\quad - \int_{\Gamma^n} (\{\nabla w\} \cdot [v] + \{\nabla v\} \cdot [w] - \sigma[w] \cdot [v]) ds. \end{aligned} \quad (\text{C.3})$$

Η μη αρνητική συνάρτηση $\sigma: \Gamma \rightarrow \mathbb{R}$ καλείται παράμετρος ποινής ασυνέχειας. Για την ανάλυση σφάλματος, είναι επιθυμητό η διγραμμική να μπορεί εφαρμοσθεί στην ακριβή λύση u . Εισάγουμε μια επέκταση της (4.12) από τον χώρο $S_h^n \times S_h^n$ στον χώρο $S^n \times S^n$, όπου $S^n := H_0^1 + S_h^n$,

$$\begin{aligned} \tilde{B}_n(w, v) &= \sum_{\tau \in \mathcal{T}_h^n} \int_{\tau} \nabla w \cdot \nabla v dx \\ &\quad - \int_{\Gamma^n} (\{\mathbf{P}_h^n \nabla w\} \cdot [v] + \{\mathbf{P}_h^n \nabla v\} \cdot [w] - \sigma[w] \cdot [v]) ds; \end{aligned} \quad (\text{C.4})$$

$\mathbf{P}_h^n: [L_2(\Omega)]^d \rightarrow [S_h^n]^d$, η ορθογώνια L_2 -προβολή στον διανυσματικό χώρο πεπερασμένων στοιχείων. Οπότε, τα ολοκληρώματα που εμπεριέχουν $\{\mathbf{P}_h^n \nabla w\}$ και $\{\mathbf{P}_h^n \nabla v\}$ είναι καλώς ορισμένα, καθώς οι όροι αυτοί είναι ίχνη των ανα στοιχείο πολυωνυμικών συναρτήσεων. Συμβολίζουμε με $A_n: S_h^n \rightarrow S_h^n$ τον ασυνεχή Galerkin Laplace τελεστή τέτοιος ώστε $(A_n w, v) = B_n(w, v) = \tilde{B}_n(w, v)$ για κάθε $w, v \in S_h^n$. Αν $w, v \in H_0^1(\Omega)$, τότε $\tilde{B}_n(w, v) = (\nabla w, \nabla v)$. Τέλος, παρατηρούμε ότι η χωρική ασυνεχής Galerkin διγραμμική μορφή (C.4) είναι συμμετρική και υπό κατάλληλη επιλογή της παραμέτρου σ είναι επίσης πιεστική.

C.2 Ανακατασκευές

Αρχικά, εισάγουμε μιας ανώτερης τάξης χρονική ανακατασκευή σε ασθενή διατύπωση. Παρουσιάζουμε δύο διαφορετικές άμεσες αναπαραστάσεις με βάση την αρχική προσέγγιση των [MN06] και τις μεταγενέστερες εργασίες των [SW10, HW17]. Το επόμενο βήμα είναι ο ορισμός μιας παραλλαγής της ελειπτικής ανακατασκευής και η μετέπειτα σύνδεσή της με την χρονική ανακατασκευή, η οποία είναι απαραίτητη για την απόδειξη των εκ των υστέρων εκτιμήσεων σφάλματος.

Χρονική ανακατασκευή

Έστω ο ακόλουθος χρονικά ημιδιακριτός χώρος

$$S_k := \left\{ V : (0, T] \rightarrow L_2(\Omega); V|_{J_n} \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)), n = 1, \dots, N \right\}. \quad (\text{C.5})$$

Θεωρούμε την χρονική ανακατασκευή $\widehat{W} := R(W)$ όπου $R: \mathbb{P}_{q_n}(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n+1}(J_n; L_2(\Omega))$ είναι ο λεγόμενος τελεστής ανακατασκευής.

Ορισμός C.2 (χρονική ανακατασκευή). Σε κάθε J_n , $n = 1, \dots, N$, ορίζουμε την χρονική ανακατασκευή $\widehat{W}|_{J_n} \in \mathbb{P}_{q_n+1}(J_n; L_2(\Omega))$ μιας συνάρτησης $W \in S_k$ έτσι ώστε να ικανοποιεί για κάθε $V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega))$, $n = 1, \dots, N$,

$$\int_{J_n} (\widehat{W}_t, V) dt = ([W]_{n-1}, V(t_{n-1}^+)) + \int_{J_n} (W_t, V) dt, \quad (C.6)$$

$$\widehat{W}(t_{n-1}^+) = W(t_{n-1}^-).$$

Στο [MN06, Section 2.1], η χρονική ανακατασκευή $\widehat{W} = R(W)$ κατασκευάζεται κατά τημήματα ως η παρεμβολή μιας συνάρτησης $W \in S_k$ στα σημεία Radau. Πράγματι, έστω $\{\widehat{\ell}_{n-1,j}\}_{j=0}^{q_n+1} \subset \mathbb{P}_{q_n+1}$ τα πολυώνυμα Lagrange που σχετίζονται με τα σημεία Radau $\{t_{n-1,j}\}_{j=0}^{q_n+1}$ στο \bar{J}_n έτσι ώστε

$$R(W)(t)|_{J_n} := \sum_{j=0}^{q_n+1} \widehat{\ell}_{n-1,j}(t) W(t_{n-1,j}),$$

να ικανοποιεί την (C.6). Από το [MN06, Lemma 2.1], προκύπτει ότι η \widehat{W} είναι καλώς ορισμένη και συνεχής στο $[0, T]$, ικανοποιώντας $\widehat{W}(t_{n-1,j}) = W(t_{n-1,j})$, για $j = 1, \dots, q_n + 1$. Συνέπεια των παραπάνω είναι η ακόλουθη αναπαράσταση:

$$(\widehat{W} - W)(t)|_{J_n} = \widehat{\ell}_{n-1,0}(t) [W]_{n-1} \quad \forall t \in J_n.$$

Ωστόσο, ο τελεστής ανακατασκευής R χρησιμοποιείται μόνο για τους σκοπούς της ανάλυσης και δεν χρειάζεται να υπολογιστεί στην πράξη. Παραθέτουμε έναν εναλλακτικό χαρακτηρισμό του σφάλματος ανακατασκευής $\widehat{W} - W$ με βάση τα [SW10, Section 4.1] και [GLW21, Section 3.3] που περιγράφουν τα άλματα του W στους χρονικούς κόμβους μέσω του τελεστή ανύψωσης. Θεωρούμε $\chi_n : L_2(\Omega) \rightarrow \mathbb{P}_{q_n}(J_n; L_2(\Omega))$, $n = 1, \dots, N$, ένα γραμμικό τελεστή χρονικής ανύψωσης ο οποίος ορίζεται για κάθε $v \in L_2(\Omega)$ μέσω

$$\int_{J_n} (\chi_n(v), V) dt = (v, V(t_{n-1}^+)) \quad \text{για κάθε } V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)). \quad (C.7)$$

Τότε, προκύπτει ο ακόλουθος χαρακτηρισμός για $t \in \bar{J}_n$

$$\widehat{W}(t)|_{J_n} = W(t_{n-1}^-) + \int_{t_{n-1}}^t (W_t(s) + \chi_n([W]_{n-1})(s)) ds,$$

που είναι ισοδύναμη με την (C.6). Επιπλέον, καταλήγουμε στον τύπο αναπαράστασης

$$(\widehat{W} - W)(t)|_{J_n} = \int_{t_{n-1}}^t \chi_n([W]_{n-1})(s) ds - [W]_{n-1}, \quad t \in \bar{J}_n. \quad (C.8)$$

Συμβολίζουμε με $\varkappa_n : J_n \rightarrow \mathbb{R}$ το πολυώνυμο βαθμού q_n , έτσι ώστε $\chi_n([V]_{n-1})(t) = \varkappa_n(t)[V]_{n-1}$ για κάθε $t \in J_n$, $V \in S_k$. Δείτε [HW17] για άμεση αναπαράσταση του \varkappa_n . Παραθέτουμε ταυτότητες σφάλματος της χρονικής ανακατασκευής:

Λήμμα C.3. [GLW21, Proposition 3.4] Έστω X χώρος Hilbert, $U|_{J_n} \in \mathbb{P}_{q_n}(J_n; X)$, $n = 1, \dots, N$ και \widehat{U} όπως ορίζεται στη (C.2). Δοθέντος $U(t_0^-) \in X$, ισχύουν

$$\begin{aligned}\|U - \widehat{U}\|_{L_2(J_n; X)} &= C_n^{1/2} \|[\![U]\!]_{n-1}\|_X, \\ \|U - \widehat{U}\|_{L_\infty(J_n; X)} &= \|[\![U]\!]_{n-1}\|_X,\end{aligned}$$

όπου $C_n := k_n(q_n + 1)/(2q_n + 1)(2q_n + 3)$.

Λήμμα C.4. Έστω $U|_{J_n} \in \mathbb{P}_{q_n}(J_n; L_p(\Omega))$, $n = 1, \dots, N$ και $2 < p < +\infty$ με \widehat{U} satisfies (C.6). Δοθέντος $U(t_0^-) \in L_p(\Omega)$, ισχύουν

$$\|\widehat{U} - U\|_{L_p(J_n; L_p(\Omega)))} \leq C \left(\frac{q_n^{p-4}}{k_n^{p-2}} \right)^{1/2p} \|[\![U]\!]_{n-1}\|_{L_p(\Omega)}.$$

Έστω $\Pi_{hk} \equiv P_h^n \pi_{q_n} : L_2(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n}(J_n; S_h^n)$, η $L_2(J_n; L_2(\Omega))$ -ορθογώνια προβολή που ορίζεται

$$\int_{J_n} (\Pi_{hk} X, V) dt = \int_{J_n} (X, V) dt, \quad \text{για κάθε } V \in \mathbb{P}_{q_n}(J_n; S_h^n),$$

όπου $\pi_{q_n} : L_2(J_n; L_2(\Omega)) \rightarrow \mathbb{P}_{q_n}(J_n; L_2(\Omega))$ τέτοιο ώστε

$$\int_{J_n} (\pi_{q_n} X, V) dt = \int_{J_n} (X, V) dt, \quad \text{για κάθε } V \in \mathbb{P}_{q_n}(J_n; L_2(\Omega)),$$

για $n = 1, \dots, N$ και P_h^n είναι η ορθογώνια L_2 -προβολή στον S_h^n .

Ελλειπτική ανακατασκευή

Έστω $U \in S_{hk}$ η προσεγγιστική λύση του (C.2) και \widehat{U} η αντίστοιχη χρονική ανακατασκευή. Επαναλαμβάνοντας τους παραπάνω συμβολισμούς είμαστε έτοιμοι να εισάγουμε την ελλειπτική ανακατασκευή και κάποιες σημαντικές ιδιότητες αυτής.

Ορισμός C.5 (ελλειπτική ανακατασκευή). Για κάθε $t \in J_n$, $n = 1, \dots, N$, ορίζουμε την ελλειπτική ανακατασκευή $\widetilde{U}(t) \in H_0^1(\Omega)$ ως εξής

$$(\nabla \widetilde{U}(t), \nabla v) = (g^n(t), v), \quad \text{για κάθε } v \in H_0^1(\Omega), \quad (\text{C.9})$$

με αρχική τιμή $\widetilde{U}(0) = \widetilde{U}(t_0^-) := u_0$ και

$$\begin{aligned}g^n(t) &:= A_n U(t) - \Pi_{hk} f(t) + \pi_{q_n} f(t) - \epsilon^{-2} \left(\pi_{q_n} F(U(t)) - \Pi_{hk} F(U(t)) \right) \\ &\quad + P_h^n \widehat{U}_t(t) - \widehat{U}_t(t).\end{aligned} \quad (\text{C.10})$$

Αρχικά, να παρατηρήσουμε ότι η έκφραση $P_h^n \widehat{U}_t - \widehat{U}_t$, η οποία εμφανίζεται στην (C.10), καλείται δείκτης αλλαγής πλέγματος. Συγκεκριμένα, σε κάθε J_n ,

$$P_h^n \widehat{U}_t - \widehat{U}_t = \varkappa_n(t) (U_{n-1}^- - P_h^n U_{n-1}^-), \quad t \in J_n,$$

όπου $U_{n-1}^- \in S_h^{n-1}$ και $P_h^n U_{n-1}^- \in S_h^n$. Επιπλέον, για κάθε $t \in J_n$, $n = 1, \dots, N$, η πλήρως διακριτή λύση $U(t)$ του (C.2) είναι επίσης η χωρική ασυνεχής Galerkin λύση

του ελλειπτικού προβλήματος (C.9). Πράγματι, έστω $\tilde{U}_h \in S_h^n$ η χωρική αυνεχής Galerkin προσέγγιση του \tilde{U} , τότε προκύπτει

$$B_n(\tilde{U}_h, V_h) = (A_n U, V_h) = B_n(U, V_h), \quad \text{για κάθε } V_h \in S_h^n,$$

το οποίο συνεπάγεται ότι $U = \tilde{U}_h$. Αυτή η παρατήρηση, μας οδηγεί στην απόδειξη εκ των υστέρων εκτιμητών σφάλματος ελλειπτικής ανακατασκευής για $p \geq 2$

$$\|\tilde{U}(t) - U(t)\|_{L_p(\Omega)} \leq \mathcal{E}(U(t), g^n(t); L_p(\Omega)) \quad \text{για κάθε } t \in J_n, \quad (\text{C.11})$$

της μορφής

$$\begin{aligned} & \mathcal{E}(U(t), g^n(t); L_p(\Omega)) \\ &= C_\Omega \left(\sum_{\tau \in \mathcal{T}_h^n} C_{I_1} \|h_\tau^2(g^n + \Delta U)\|_{L_p(\tau)}^p + \sum_{e \in \Gamma_{int}^n} C_{I_2} \|h_\tau^{1+1/p} [\nabla U]\|_{L_p(e)}^p \right. \\ & \quad \left. + \sum_{e \in \Gamma^n} C_{I_3} \|h_\tau^{1/p} [U]\|_{L_p(e)}^p + \sum_{e \in \Gamma^n} C_{I_4} \sigma^p \|h_\tau^{1+1/p} [U]\|_{L_p(e)}^p \right)^{1/p}. \end{aligned}$$

Τέλος, η χρονική ανακατασκευή της ασυνεχούς Galerkin λύσης U επιτρέπει την επαναδιατύπωση του (C.2) σε ισχυρή μορφή. Ταυτόχρονα, προκύπτει μια άμεση συσχέτιση της χρονικής ανακατασκευής με την ελλειπτική ανακατασκευή: Για κάθε $n = 1, \dots, N$ έχουμε την ακόλουθη σημειακή αναπαράσταση

$$\hat{U}_t(t) - \Delta \tilde{U}(t) + \epsilon^{-2} \pi_{q_n} F(U(t)) = \pi_{q_n} f(t), \quad \text{για κάθε } t \in J_n. \quad (\text{C.12})$$

C.3 Εκ των υστέρων εκτιμήσεις σφάλματος

Αποδεικνύουμε εκ των υστέρων εκτιμήσεις σφάλματος στις $L_4(0, T; L_4(\Omega))$ -, $L_\infty(0, T; L_2(\Omega))$ - και $L_2(0, T, H^1(\Omega))$ -νόρμες συνδυάζοντας την χωροχρονική ανακατασκευή με επιχειρήματα συνέχειας και μια ‘βελτιωμένη’ φασματική εκτίμηση για γραμμικοποιημένο τελεστή Allen-Cahn ως προς την προσεγγιστική λύση $U(t)$. Έστω $\omega := \hat{\tilde{U}}$ η χρονική ανακατασκευή της ελλειπτικής ανακατασκευής, ισχύει διότι $\tilde{U} \in S_k$. Διασπάμε το ολικό σφάλμα όπως στο [GLW21]:

$$e := u - U = \theta - \rho, \quad \text{όπου } \theta := \omega - U, \quad \rho := \omega - u.$$

Εναλλακτικά γράφουμε, $\theta := \omega - U = (\hat{\tilde{U}} - \tilde{U}) + (\tilde{U} - U)$; ως σφάλμα χρονικής ανακατασκευής και σφάλμα ελλειπτικής ανακατασκευής, δηλαδή για $p \geq 2$ έχουμε,

$$\|\theta\|_{L_p(\Omega)} \leq \|\hat{\tilde{U}} - \tilde{U}\|_{L_p(\Omega)} + \|\tilde{U} - U\|_{L_p(\Omega)};$$

Αρκεί να εκτιμήσουμε το ρ ως προς το θ και τα δεδομένα του προβλήματος. Οι σχέσεις (3.1), (C.12) και στοιχειώδεις πράξεις οδηγούν στο ακόλουθο λήμμα:

Λήμμα C.6 (εξίσωση σφάλματος). Σε κάθε J_n , $n = 1, \dots, N$ και για όλα τα $v \in H_0^1(\Omega)$, ισχύει,

$$\begin{aligned} & (\rho_t, v) + (\nabla \rho, \nabla v) + \epsilon^{-2} (F(U) - F(u), v) \\ &= (\pi_{q_n} f - f, v) + ((\omega - \hat{\tilde{U}})_t, v) + (\nabla(\omega - \tilde{U}), \nabla v) \\ & \quad + \epsilon^{-2} (F(U) - \pi_{q_n} F(U), v). \end{aligned} \quad (\text{C.13})$$

Εισάγουμε ορισμένους συμβολισμούς: σε κάθε J_n , $n = 1, \dots, N$ ορίζουμε

$$\begin{aligned}\mathcal{L}_1^{\text{dG}}(t) &:= \|\Delta(\omega - \tilde{U})\|_{L_2(\Omega)}^2, \\ \mathcal{L}_2^{\text{dG}}(t) &:= \|\pi_{q_n} f - f\|_{L_2(\Omega)}^2 + \epsilon^{-4} \|F(U) - \pi_{q_n} F(U)\|_{L_2(\Omega)}^2,\end{aligned}$$

Επιπλέον, θέτουμε $C_0 := (C_P \tilde{c}^2 + 1)/2$, $C_1 := (9C_P \tilde{c}^2 + 6^6 C_P^2 \tilde{c}^4 + 3^7 2^{-4} \epsilon^2 + 9)/2$, $C_2 := 3^7 C_P^2 \tilde{c}^4 + 3^7 (1 + C_P^2)^2 \tilde{c}^4$, C_P η σταθερά της (2.8), $\hat{\epsilon}$ σταθερά ενσφήνωσης $\|v\|_{L_8(\Omega)} \leq \hat{\epsilon} \|v\|_{H^1(\Omega)}$ και \tilde{c} όπως στις (2.3)-(2.5), έτσι ώστε

$$\begin{aligned}\Theta_1^{\text{dG}}(t) &:= \frac{1}{2} \|(\omega - \tilde{U})_t\|_{L_2(\Omega)}^2 + \frac{3C_P^4}{2} \|(\omega - \tilde{U})_t\|_{L_4(\Omega)}^4, \\ \Theta_2^{\text{dG}}(t) &:= \epsilon^{-4} \left((C_0 + 216 \|U\|_{L_\infty(\Omega)}^2) \|\theta\|_{L_2(\Omega)}^2 + C_1 \|\theta\|_{L_4(\Omega)}^4 + C_0 \|\theta\|_{L_6(\Omega)}^6 \right), \\ A^{\text{dG}}(t) &:= \epsilon^{-2} \left((\theta^2 \rho^2 + \rho^4 + |\nabla \rho|^2, \int_t^\tau \rho^2(s) \, ds) + (\theta^2, \rho^2) \right);\end{aligned}$$

Θ_1 εκφράζει το σφάλμα χωρικής ανακατασκευής και Θ_2 (ή $\tilde{\Theta}_2$ όταν $d = 3$) δηλώνει τις εκτιμήσεις χωρικών σφαλμάτων, λόγω της παρουσίας των διαφόρων νορμών των όρων θ και $(\omega - \tilde{U})_t$. Αναλύουμε το τελευταίο όρο προκειμένου να δικαιολογήσουμε αυτόν τον χαρακτηρισμό. Λαμβάνοντας υπόψη το (C.2), έχουμε

$$\|(\omega - \tilde{U})_t\|_{L_p(\Omega)} \leq \|\tilde{U}_t - U_t\|_{L_p(\Omega)} + |\varkappa_n(t)| \|\tilde{U} - U\|_{n-1} \|_{L_p(\Omega)}, \quad t \in J_n,$$

όπου $\|\tilde{U} - U\|_{n-1} = (\tilde{U} - U)(t_{n-1}^+ - (\tilde{U} - U)(t_{n-1}^-)$. Διαφορίζουμε την (4.26) ως προς τη χρονική μεταβλητή, καταλήγουμε σε μια σχέση αντίτοιχη της (C.2) που συνεπάγεται ότι η U_t είναι η ασυνεχής χωρική Galerkin προσέγγιση του \tilde{U}_t . Εχοντας εκτιμητές της μορφής (C.11), έπειτα για $U_{n-1}^- \in S_h^{n-1}$ και $U_{n-1}^+ \in S_h^n$

$$\begin{aligned}\|(\omega - \tilde{U})_t\|_{L_p(\Omega)} &\leq \mathcal{E}(U_t, g_t^n(t); L_p(\Omega)) + |\varkappa_n(t)| \mathcal{E}(U_{n-1}^-, g^{n-1}(t_{n-1}^-); L_p(\Omega)) \\ &\quad + |\varkappa_n(t)| \mathcal{E}(U_{n-1}^+, g^n(t_{n-1}^+); L_p(\Omega)), \quad t \in J_n.\end{aligned}$$

Σε αυτό το σημείο, παρασοιάζουμε δύο Λήμματα αντίστοιχα των B.4 και B.5.

Λήμμα C.7 ($d = 2$). Έστω $d = 2$ και u η λύση της (3.1). Υποθέτουμε ότι $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ για σ.κ. $t \in (0, T]$. Τότε, για κάθε $\tau \in (0, T]$, έχουμε

$$\begin{aligned}&\frac{1}{8} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 \, dt + \frac{1}{8} \int_0^\tau \|\nabla \rho^2(s)\|_{L_2(\Omega)}^2 \, ds + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ &\quad + \int_0^\tau A^{\text{dG}}(t) \, dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2} \right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U)\rho, \rho) \right) \, dt \\ &\leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1^{\text{dG}} + \Theta_2^{\text{dG}} + C_0(\mathcal{L}_1^{\text{dG}} + \mathcal{L}_2^{\text{dG}})) \, dt \quad (\text{C.14}) \\ &\quad + \frac{1}{2} \int_0^\tau \left(\int_t^\tau \|\nabla \rho^2(s)\|_{L_2(\Omega)}^2 \, ds + \alpha^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^2 \right) \, dt \\ &\quad + \frac{1}{4\epsilon^6} \int_0^\tau \left(\beta^{\text{dG}}(\theta, U) \int_t^\tau \|\nabla \rho^2(s)\|_{L_2(\Omega)}^4 \, ds + \gamma^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^4 \right) \, dt,\end{aligned}$$

όπου

$$\begin{aligned}\alpha^{\text{dG}}(U) &:= \|F'(U)\|_{L_\infty(\Omega)}^2 + \|U\|_{L_\infty(\Omega)}^2 + 5 \\ \beta^{\text{dG}}(\theta, U) &:= C_2 \epsilon^4 (\|\theta\|_{L_8(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4) + 2\epsilon^2 \|U\|_{L_\infty(\Omega)}^4 \\ &\quad + 2C_P^2 \tilde{c}^4 \|F'(U)\|_{L_\infty(\Omega)}^2 + 6\epsilon^6 (\|F'(U)\|_{L_\infty(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4 + 4), \\ \gamma^{\text{dG}}(U) &:= 2\tilde{c}^4 (C_P^2 \|F'(U)\|_{L_\infty(\Omega)}^2 + 18 \|U\|_{L_\infty(\Omega)}^2).\end{aligned}$$

Λήμμα C.8 ($d = 3$). Έστω $d = 3$ και u η λύση της (3.1). Υποθέτουμε ότι $\rho(t) \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ για σ.κ. $t \in (0, T]$. Τότε, για κάθε $\tau \in (0, T]$, έχουμε

$$\begin{aligned}&\frac{1}{16} \int_0^\tau \|\rho\|_{L_4(\Omega)}^4 dt + \frac{1}{8} \left\| \int_0^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + \frac{1}{2} \|\rho(\tau)\|_{L_2(\Omega)}^2 \\ &+ \int_0^\tau A^{\text{dG}}(t) dt + \int_0^\tau \left(\left(1 - \frac{\epsilon^2}{2}\right) \|\nabla \rho\|_{L_2(\Omega)}^2 + \frac{1}{\epsilon^2} (F'(U)\rho, \rho) \right) dt \quad (\text{C.15}) \\ &\leq \frac{1}{2} \|\rho(0)\|_{L_2(\Omega)}^2 + \frac{C_P^2}{2} \|\rho(0)\|_{L_4(\Omega)}^4 + \int_0^\tau (\Theta_1^{\text{dG}} + \tilde{\Theta}_2^{\text{dG}} + \tilde{C}_0(\mathcal{L}_1^{\text{dG}} + \mathcal{L}_2^{\text{dG}})) dt \\ &+ \frac{1}{2} \int_0^\tau \left(\left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^2 + (\alpha^{\text{dG}}(U) + 1) \|\rho\|_{L_2(\Omega)}^2 \right) dt \\ &+ \frac{1}{4\epsilon^{10}} \int_0^\tau \left(\tilde{\beta}^{\text{dG}}(\theta, U) \left\| \int_t^\tau \nabla \rho^2(s) ds \right\|_{L_2(\Omega)}^4 + \tilde{\gamma}^{\text{dG}}(U) \|\rho\|_{L_2(\Omega)}^4 \right) dt,\end{aligned}$$

όπου

$$\begin{aligned}\tilde{\Theta}_2^{\text{dG}}(t) &:= \epsilon^{-4} \left((\tilde{C}_0 + 216 \|U\|_{L_\infty(\Omega)}^2) \|\theta\|_{L_2(\Omega)}^2 + \tilde{C}_1 \|\theta\|_{L_4(\Omega)}^4 + \tilde{C}_0 \|\theta\|_{L_6(\Omega)}^6 \right), \\ \tilde{\beta}^{\text{dG}}(\theta, U) &:= 3^7 \epsilon^8 (\hat{C}^4 \|\theta\|_{L_{12}(\Omega)}^4 + C_P \tilde{c}^4 \|U\|_{L_\infty(\Omega)}^4) + 2\epsilon^6 \|U\|_{L_\infty(\Omega)}^4 \\ &\quad + 4C_P \tilde{c}^4 \epsilon^2 \|F'(U)\|_{L_\infty(\Omega)}^4 + 6\epsilon^{10} (\|F'(U)\|_{L_\infty(\Omega)}^4 + \|U\|_{L_\infty(\Omega)}^4 + 4), \\ \tilde{\gamma}^{\text{dG}}(U) &:= 81C_P \tilde{c}^4 \|U\|_{L_\infty(\Omega)}^4,\end{aligned}$$

με $\tilde{C}_0 := (C_P^{1/2} \tilde{c}^2 + 1)/2$, $\tilde{C}_1 := (9 + 9C_P^{1/2} \tilde{c}^2 + 6^6 C_P \tilde{c}^4 + 2^{-1} 3^7 \epsilon^2)/2$, \hat{C} σταθερά ενσφήνωσης $\|v\|_{L_6(\Omega)} \leq \hat{C} \|\nabla v\|_{L_2(\Omega)}$.

Αν ισχύει οποιαδήποτε περίπτωση της Υπόθεσης 3.11, έχουμε ότι

$$\begin{aligned}&\|\nabla \rho\|_{L_2(\Omega)}^2 + \epsilon^{-2} (F'(U)\rho, \rho) \\ &\geq -\bar{\Lambda}(t)(1 - \epsilon^2) \|\rho\|_{L_2(\Omega)}^2 + \epsilon^2 \|\nabla \rho\|_{L_2(\Omega)}^2 + (F'(U)\rho, \rho). \quad (\text{C.16})\end{aligned}$$

Εισάγοντας το (C.16) στο (C.7) και στο (C.8) για $d=2$ και 3, αντίστοιχα, και εφαρμόζοντας ένα επιχείρημα συνέχειας είμαστε σε θέση να καταλήξουμε σε ένα ανάλογο αποτέλεσμα με το Λήμμα B.6. Με την μόνη διαφορά ότι έχουμε: για $d = 2$,

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

$$\begin{aligned}\mathcal{D}_2^{\text{dG}} &:= \max\{4, \alpha^{\text{dG}}(U) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 2\}, \mathcal{B}_2^{\text{dG}} := \max\{16\beta^{\text{dG}}(\theta, U), \gamma^{\text{dG}}(U)\}, \\ \mathcal{B}_2^{\text{dG}} &:= \sup_{t \in [0, T]} \mathcal{B}_2^{\text{dG}}(t), \text{ ενώ για } d=3,\end{aligned}$$

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

$$\mathcal{D}_3^{\text{dG}} := \max\{4, \alpha^{\text{dG}}(U) + 2\bar{\Lambda}(t)(1 - \epsilon^2) + 3\}, \quad \mathcal{B}_3^{\text{dG}} := \max\{16\tilde{\beta}^{\text{dG}}(\theta, U), \tilde{\gamma}^{\text{dG}}(U)\}, \\ \text{και } \tilde{\mathcal{B}}_3^{\text{dG}} := \sup_{t \in [0, T]} \mathcal{B}_3^{\text{dG}}(t).$$

Η ανάλογη υπό συνθήκη εκ των υστέρων εκτίμηση σφάλματος στην $L_4(0, T; L_4(\Omega))$ -νόρμα προκύπτει εφαρμόζοντας την τριγωνική ανισότητα:

Θεώρημα C.9. Έστω $u_0 \in W^{1,4}(\Omega) \cap H_0^1(\Omega)$ και $f \in L_\infty(0, T; L_4(\Omega))$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. Έστω u η λύση της (3.1) και U η προσέγγιση της (C.2). Τότε, σύμφωνα με την υπόθεση (3.11)(II) και τη συνθήκη

$$\eta_d^{\text{dG}} \leq (16(T+1)\tilde{\mathcal{B}}_d^{\text{dG}}(E_d^{\text{dG}})^2)^{-1/4} \epsilon^{d-1/2} \quad (\text{C.17})$$

ισχύει η ακόλουθη εκτίμηση

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

Σύμφωνα με τις [Che94, MS95] όταν οι διεπιφάνειες είναι ομαλές, περιμένουμε ότι $E_d^{\text{DG}} \sim 1$. Στην περίπτωση των τοπολογικών αλλαγών, με βάση το [BMO11], έχουμε ότι $E_d^{\text{DG}} \sim \epsilon^{-m}$, $m > 0$. Ειδικότερα, το E_d^{DG} δεν αυξάνεται εκθετικά στο $1/\epsilon$. Θέτοντας $C_d^{\text{dG}} := (16(T+1)\tilde{\mathcal{B}}_d^{\text{dG}})^{-1/4}$, η συνθήκη (C.17) γράφεται

$$\eta_d^{\text{dG}} \leq C_d^{\text{dG}} \epsilon^{d+(m-1)/2}, \quad \text{για } d = 2, 3, \text{ και, } m \geq 0$$

λαμβάνοντας υπόψη και τις δύο περιπτώσεις της Υπόθεσης 3.11 σχετικά με τη ύπαρξη και τις ιδιότητες ενός κάτω φράγματος, $-\Lambda$, της κυρίαρχης ιδιοτιμής.

Τέλος, όπως και στο Κεφάλαιο 3 προκύπτουν άμμεσα και οι εκτιμήσεις σφάλματος:

Πρόταση C.10. Με τις υποθέσεις του Θεωρήματος C.9 και υποθέτοντας τη συνθήκη (C.17) που συνεπάγεται

$$\hat{\eta}_d^{\text{dG}} := (\eta_d^{\text{dG}})^2 \leq (G_d^{\text{dG}})^2 \epsilon^{2d-1+m},$$

ισχύουν οι εκτιμήσεις

$$\|u - U\|_{L_\infty(0, T; L_2(\Omega))} \leq 2\sqrt{2E_d^{\text{dG}}} \hat{\eta}_d^{\text{dG}} + \|\theta\|_{L_\infty(0, T; L_2(\Omega))}, \\ \|u - U\|_{L_2(0, T; H^1(S))} \leq \epsilon^{-1} 2\sqrt{2E_d^{\text{dG}}} \hat{\eta}_d^{\text{dG}} + \|\theta\|_{L_2(0, T; H^1(S))},$$

όπου $S := S_h + H_0^1(\Omega)$.

D Κεφάλαιο 5

Το Κεφάλαιο 5 ασχολείται με την ελαχιστοποίηση του συναρτησιακού

$$J(u) = \frac{1}{2} \int_0^T \int_\Omega |y_u(t, x) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_\Omega |y_u(T, x) - y_\Omega(x)|^2 dx \\ + \frac{\mu}{2} \int_0^T \int_\Omega |u(t, x)|^2 dx dt, \quad (\text{D.1})$$

υπό την προϋπόθεση ότι

$$y_{u,t} - \Delta y_u + \frac{1}{\epsilon^2} (y_u^3 - y_u) = u \quad \text{στο } \Omega_T = \Omega \times (0, T), \\ y_u = 0 \quad \text{στο } \Sigma_T = \partial\Omega \times (0, T), \\ y_u(\cdot, 0) = y_0 \quad \text{στο } \Omega. \quad (\text{D.2})$$

Παρουσιάζουμε μια λεπτομερή ανάλυση του προβλήματος βέλτιστου ελέγχου που διατυπώνεται ως

$$\left\{ \begin{array}{l} \min J(u) \\ u \in U_{ad}, \end{array} \right. \quad (\text{D.3})$$

όπου

$$U_{ad} = \left\{ u \in L_2(0, T; L_2(\Omega)) ; u_a \leq u(t, x) \leq u_b \text{ για σ.κ. } (t, x) \in \Omega_T \right\},$$

Αρχικά, παρουσιάζουμε μια ανάλυση των απεικονίσεων ελέγχου προς την κατάσταση και της κατάστασης προς την συζυγή κατάσταση και δείχνουμε συνθήκες βελτιστοποίησης πρώτης και δεύτερης τάξης. Συγκεκριμένα, υπό την υπόθεση της εγγύτητας των ελέγχων, διαπιστώνουμε τη συνέχεια Lipschitz της απεικόνισης ελέγχου προς κατάσταση, με σταθερά Lipschitz που είναι ανεξάρτητη από το ϵ στη $L_\infty(0, T; L_2(\Omega))$ -νόρμα εκμεταλλευόμενοι την παρουσία του κρίσμου όρου στην $L_4(0, T; L_4(\Omega))$ -νόρμα, την φασματική εκτίμηση και το μη γραμμικό Λήμμα Gronwall. Για την απεικόνιση της κατάστασης προς την συζυγή κατάσταση, χρησιμοποιώντας παρόμοια τεχνικά εργαλεία είμαστε σε θέση να λάβουμε αποτελέσματα Lipschitz με σταθερές που εξαρτώνται πολυωνυμικά από το $1/\epsilon$.

D.1 Συνθήκες βελτιστοποίησης

Δεδομένου ότι έχουμε να κάνουμε με ένα μη κυρτό πρόβλημα βέλτιστου ελέγχου, οι αναγκαίες συνθήκες βελτιστοποίησης πρώτης τάξης δεν είναι πλέον ικανές. Συνεπώς, πρέπει να εξετάσουμε ικανές συνθήκες δεύτερης τάξης για την τοπική βέλτιστη λύση. Πριν από αυτό, θα διατυπώσουμε ασθενώς το (D.2) και θα παρουσιάσουμε χρήσιμα για τη συνέχεια αποτελέσματα ευστάθειας.

Υποθέτουμε ότι $u \in L_2(0, T; L_2(\Omega))$, $y_0 \in L_2(\Omega)$, $y_\Omega \in H_0^1(\Omega)$. Η ασθενής διατύπωση της εξίσωσης κατάστασης (D.2) είναι: αναζητούμε $y \in W(0, T)$ έτσι ώστε για σ.κ. $t \in (0, T)$,

$$\begin{aligned} \langle y_t, v \rangle + (\nabla y, \nabla v) + \epsilon^{-2} (y^3 - y, v) &= (u, v), \\ (y(0), v) &= (y_0, v), \end{aligned} \quad (\text{D.4})$$

για όλα τα $v \in H_0^1(\Omega)$. Για κάθε $\epsilon > 0$, και $y_0 \in H_0^1(\Omega)$, είναι εύκολο να δείξουμε ότι $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ (βλ. [Tem97]). Το ακόλουθο λήμμα προσδιορίζει την εξάρτηση από το ϵ διαφόρων νορμών.

Λήμμα D.1. 1. Έστω $u \in L_2(0, T; L_2(\Omega))$ και $y_0 \in L_2(\Omega)$. Τότε, υπάρχει μια σταθερά C ανεξάρτητη από το ϵ τέτοια ώστε:

$$\begin{aligned} &\|y\|_{L_2(0, T; L_2(\Omega))} + \|y\|_{L_4(0, T; L_4(\Omega))}^2 \\ &\leq C \left(|\Omega_T|^{\frac{1}{2}} + \epsilon \|y_0\|_{L_2(\Omega)} + \epsilon^2 \|u\|_{L_2(0, T; L_2(\Omega))} \right) =: C_{st,1}, \\ &\|y\|_{L_\infty(0, T; L_2(\Omega))} + \|y\|_{L_2(0, T; H^1(\Omega))} \leq \frac{C_{st,1}}{\epsilon}. \end{aligned}$$

2. Έστω $u \in L_2(0, T; L_2(\Omega))$ και $y_0 \in H_0^1(\Omega)$. Τότε, υπάρχει μια σταθερά C

ανεξάρτητη από το ϵ , ώστε να ισχύουν οι ακόλουθες εκτιμήσεις:

$$\begin{aligned} & \|y\|_{L_\infty(0,T;H^1(\Omega))} + \|y_t\|_{L_2(0,T;L_2(\Omega))} + \frac{1}{2\epsilon} \|(y^2 - 1)^2\|_{L_\infty(0,T;L_1(\Omega))}^{1/2} \\ & \leq C \left(\|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{st,2}, \\ & \|y\|_{L_2(0,T;H^2(\Omega))} \leq C \left(\frac{T^{1/2}C_{st,2}}{\epsilon} + \|\nabla y_0\|_{L_2(\Omega)} + \|u\|_{L_2(0,T;L_2(\Omega))} \right) := C_{st,3}. \end{aligned}$$

Παρατηρούμε ότι αν

$$\|\nabla y(0)\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y^2(0) - 1)^2\|_{L_1(\Omega)}^{1/2} \leq D,$$

με D ανεξάρτητη του ϵ , τότε ισχύει ότι η $C_{st,2}$ φράσσεται ανεξάρτητα του ϵ και συνεπώς συμπεραίνουμε ότι

$$\|y\|_{H^{2,1}(\Omega_T)} \leq \frac{C}{\epsilon} (D + \|u\|_{L_2(0,T;L_2(\Omega))}),$$

όπου C είναι μια αλγεβρική σταθερά που εξαρτάται μόνο από το χωρίο.

Συνέχεια

Ξεκινάμε με τη μελέτη της συνέχειας της σχέσης ελέγχου-κατάστασης και δίνεται έμφαση στην εξάρτηση από το ϵ των διαφόρων σταθερών Lipschitz.

Ορισμός D.2. Η απεικόνιση $G : L_2(0, T; L_2(\Omega)) \rightarrow H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ που αντιστοιχίζει κάθε συνάρτηση ελέγχου u στην κατάσταση $y_u = y(u) = G(u)$, ονομάζεται τελεστής ελέγχου προς την κατάσταση.

Για $u_i \in L_2(0, T; L_2(\Omega))$, $i = 1, 2$, συμβολίζουμε με $y_i = G(u_i) := y_{u_i}$.

Θεώρημα D.3. Υποθέτουμε ότι ισχύει,

$$\begin{aligned} \|u_1 - u_2\|_{L_2(0,T:L_2(\Omega))} & \leq \frac{\epsilon^3 \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{-1}}{12\tilde{c}(T+1)} E^{-1}, \quad \text{για } d = 2, \\ \|u_1 - u_2\|_{L_2(0,T:L_2(\Omega))} & \leq \frac{\epsilon^4 \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{-1}}{48\tilde{c}(T+1)} E^{-3/2}, \quad \text{για } d = 3, \end{aligned} \tag{D.5}$$

όπου $E := \exp(\int_0^T 2\lambda(t)(1-\epsilon^2) + (6-d) dt)$. Τότε, υπάρχει σταθερά $L_1 := 2E^{1/2}$, τέτοια ώστε

$$\begin{aligned} & \sup_{t \in [0, T]} \|y_1 - y_2\|_{L_2(\Omega)} + \epsilon \|y_1 - y_2\|_{L_2(0,T;H_0^1(\Omega))} + \epsilon^{-1} \|y_1 - y_2\|_{L_4(0,T;L_4(\Omega))}^2 \\ & \leq L_1 \|u_1 - u_2\|_{L_2(0,T:L_2(\Omega))}. \end{aligned} \tag{D.6}$$

Παραγωγισμότητα

Προσδιορίζουμε τις παραγώγους πρώτης και δεύτερης τάξης του G , οι οποίες παίζουν καθοριστικό ρόλο στην απόδειξη των συνθηκών βελτιστοποίησης. Σε αυτό το βήμα, είναι απαραίτητη η ανάλυση της εξίσωσης συζυγούς κατάστασης.

Θεώρημα D.4. Έστω $u, v \in L_2(0, T; L_2(\Omega))$. Η απεικόνιση $G : L_2(0, T; L_2(\Omega)) \rightarrow H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$, ώστε $y_u = G(u)$, είναι της τάξης C^∞ . Συμβολίζουμε με $z_v = G'(u)v$ και $z_{vv} = G''(u)v^2$, τις μοναδικές λύσεις των ακόλουθων εξισώσεων

$$\begin{aligned} z_{v,t} - \Delta z_v + \epsilon^{-2} (3y_u^2 - 1) z_v &= v \quad \text{στο } \Omega_T, \\ z_v &= 0 \quad \text{στο } \Sigma_T, \quad z_v(0) = 0 \quad \text{στο } \Omega, \end{aligned} \tag{D.7}$$

$$\begin{aligned} z_{vv,t} - \Delta z_{vv} + \epsilon^{-2} (3y_u^2 - 1) z_{vv} &= -6\epsilon^{-2} y_u z_v^2 \quad \text{στο } \Omega_T, \\ z_{vv} &= 0 \quad \text{στο } \Sigma_T, \quad z_{vv}(0) = 0 \quad \text{στο } \Omega. \end{aligned} \tag{D.8}$$

Οι ιδιότητες παραγωγισμότητα του G συνεπάγονται ότι η συνάρτηση κόστους $J : L_2(0, T; L_2(\Omega)) \rightarrow \mathbb{R}$ είναι επίσης κλάσης C^∞ .

Λήμμα D.5. Για κάθε $u, v \in L_2(0, T; L_2(\Omega))$, ισχύει ότι

$$J'(u)v = \int_0^T \int_\Omega (\varphi_u + \mu u)v \, dx \, dt, \tag{D.9}$$

$$\begin{aligned} J''(u)v^2 &= \int_0^T \int_\Omega |z_v|^2 \, dx \, dt + \gamma \int_\Omega |z_v(T)|^2 \, dx + \mu \int_0^T \int_\Omega |v|^2 \, dx \, dt \\ &\quad - 6\epsilon^{-2} \int_0^T \int_\Omega y_u z_v^2 \varphi_u \, dx \, dt, \end{aligned} \tag{D.10}$$

όπου z_v έιναι η λύση του (D.7) ενώ $\varphi_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ είναι η μοναδική λύση που ικανοποιεί για κάθε $w \in H_0^1(\Omega)$ την εξισωση συζυγούς κατάστασης,

$$\begin{aligned} -(\varphi_{u,t}, w) + (\nabla \varphi_u, \nabla w) + \epsilon^{-2} ((3y_u^2 - 1) \varphi_u, w) &= (y_u - y_d, w) \\ \varphi_u(T) &= \gamma(y_u(T) - y_\Omega). \end{aligned} \tag{D.11}$$

Λήμμα D.6. Έστω φ_u λύση του (D.11), $y_d \in L_2(0, T; L_2(\Omega))$ και $\varphi_u(T) \in H_0^1(\Omega)$. Τότε, υπάρχει αλγεβρική σταθερά $C > 0$, που εξαρτάται μόνο από Ω έτσι ώστε

$$\begin{aligned} &\sup_{t \in [0, T]} \|\varphi_u(t)\|_{L_2(\Omega)} + \epsilon \|\nabla \varphi_u\|_{L_2(0, T; L_2(\Omega))} + \|\varphi_u y_u\|_{L_2(0, T; L_2(\Omega))} \\ &\leq CC_\varphi^{1/2} \left(\|\varphi_u(T)\|_{L_2(\Omega)} + \|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} \right) := D_{st,1}, \end{aligned} \tag{D.12}$$

$$\begin{aligned} &\|\varphi_{u,t}\|_{L_2(0, T; L_2(\Omega))} + \sup_{t \in [0, T]} \|\nabla \varphi_u(t)\|_{L_2(\Omega)} \\ &\leq C \left(\|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} + \frac{1}{\epsilon^2} \left(\|y_u\|_{L_\infty(0, T; L_\infty(\Omega))} + T^{1/2} D_{st,1} \right) \right. \\ &\quad \left. + \|\nabla \varphi_u(T)\|_{L^2(\Omega)} \right) := D_{st,2}, \end{aligned} \tag{D.13}$$

$$\|\varphi_u\|_{L_2(0, T; H^2(\Omega))} \tag{D.14}$$

$$\leq C \left(\|y_u - y_d\|_{L_2(0, T; L_2(\Omega))} + D_{st,2} + \frac{1}{\epsilon^2} (1 + 3\|y_u\|_{L_\infty(0, T; L_\infty(\Omega))}) D_{st,1} \right),$$

όπου $C_\varphi := \exp \left(\int_0^T (2\lambda(t)(1 - \epsilon^2) + 3) \, dt \right)$.

Έστω $u_1, u_2 \in L_2(0, T; L_2(\Omega))$ οι συναρτήσεις ελέγχου και $y_i = y_{u_i}$, $\varphi_i = \varphi_{u_i}$ οι λύσεις κατάστασης και συζυγούς κατάστασης για $i = 1, 2$, αντίστοιχα.

Λήμμα D.7. Υποθέτουμε ότι η (D.5) ισχύει. Τότε, για $d = 2$, υπάρχει σταθερά C_T που εξαρτάται μόνο από το Ω_T έτσι ώστε,

$$\begin{aligned} & \sup_{t \in [0, T]} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)} + \epsilon \|\varphi_1 - \varphi_2\|_{L_2(0, T; H_0^1(\Omega))} \\ & \leq C_T E_\varphi^{1/2} L_1 \left(1 + \frac{C_\infty \tilde{c} D_{st,1}}{\epsilon^{7/2}} \right) \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))}. \end{aligned} \quad (\text{D.15})$$

Για $d = 3$, υπάρχει σταθερά C_T που εξαρτάται μόνο από το Ω_T έτσι ώστε,

$$\begin{aligned} & \sup_{t \in [0, T]} \|\varphi_1 - \varphi_2\|_{L_2(\Omega)} + \epsilon \|\varphi_1 - \varphi_2\|_{L_2(0, T; H_0^1(\Omega))} \\ & \leq C_T E_\varphi^{1/2} L_1 \left(1 + \frac{C_\infty \tilde{c} D_{st,1}}{\epsilon^{15/4}} \right) \|u_1 - u_2\|_{L_2(0, T; L_2(\Omega))}, \end{aligned} \quad (\text{D.16})$$

Εδώ, συμβολίζουμε με $C_\infty := \left(C(\|y_1\|_{L_\infty(0, T; L_\infty(\Omega))}^2 + \|y_2\|_{L_\infty(0, T; L_\infty(\Omega))}^2) \right)^{1/2}$ με C να εξαρτάται από το $|\Omega|$, και $E_\varphi := \int_0^T (2\lambda(t)(1 - \epsilon^2) + 4) dt$.

Ανογκαίες και ικανές συνθήκες

Παρακάτω, αναφέρουμε τις συνθήκες βελτιστοποίησης. Για τις σχετικές αποδείξεις παραπέμπουμε τους αναγνώστες στο [CC12, Theorems 3.4 και 3.3].

Θεώρημα D.8. Κάθε τοπικά βέλτιστος έλεγχος \bar{u} για το πρόβλημα (D.3), ικανοποιεί, μαζί με τη αντίστοιχη κατάσταση $\bar{y} \in H^{2,1}(\Omega_T)$ για δόλα τα $v \in H_0^1(\Omega)$

$$\begin{cases} (\bar{y}_t, v) + (\nabla \bar{y}, \nabla v) + \epsilon^{-2} (\bar{y}^3 - \bar{y}, v) = (\bar{u}, v) \\ \bar{y}(0) = y_0, \end{cases} \quad (\text{D.17})$$

και την συζυγή κατάσταση $\bar{\varphi} \in H^{2,1}(\Omega_T)$ για δόλα τα $w \in H_0^1(\Omega)$

$$\begin{cases} -(\bar{\varphi}_t, w) + (\nabla \bar{\varphi}, \nabla w) + \epsilon^{-2} ((3\bar{y}^2 - 1)\bar{\varphi}, w) = (\bar{y} - y_d, w) \\ \bar{\varphi}(T) = \gamma(\bar{y}(T) - y_\Omega), \end{cases} \quad (\text{D.18})$$

την ανισότητα μεταβολής (συνθήκη βελτιστοποίησης)

$$\int_0^T \int_\Omega (\bar{\varphi} + \mu \bar{u}) (u - \bar{u}) dx dt \geq 0 \quad \forall u \in U_{ad}, \quad (\text{D.19})$$

με $\bar{u} \in L_2(0, T; W^{1,p}(\Omega)) \cap C(0, T; H^1(\Omega)) \cap H^1(\Omega_T)$, για οποιοδήποτε $1 \leq p < \infty$. Επιπλέον, έστω $\epsilon \|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq C$. Τότε,

$$\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C} \epsilon^{-2}, \quad \text{και} \quad \|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D} \epsilon^{-3}.$$

Αν ακόμη, $\|\nabla y_0\|_{L_2(\Omega)} + \frac{1}{2\epsilon} \|(y_0^2 - 1)^2\|_{L_1(\Omega)}^{1/2} \leq D$ τότε,

$$\|\bar{y}\|_{H^{2,1}(\Omega_T)} \leq \tilde{C} \epsilon^{-1}, \quad \text{και} \quad \|\bar{\varphi}\|_{H^{2,1}(\Omega_T)} \leq \tilde{D} \epsilon^{-2};$$

οι σταθερές \tilde{C}, \tilde{D} είναι ανεξάρτητες από το ϵ και εξαρτώνται μόνο από τα δεδομένα.

Η ανισότητα (D.19) συνεπάγεται των κλασικό τύπο προβολής

$$\bar{u}(t, x) = \text{Proj}_{[u_a, u_b]} \left(-\frac{1}{\mu} \bar{\varphi}(t, x) \right) \text{ για } \sigma.\pi. (t, x) \in \Omega_T. \quad (\text{D.20})$$

Με τον συνήθη τρόπο, συμπεραίνουμε από το (5.27) ότι για σ.κ. $(t, x) \in \Omega_T$,

$$\begin{cases} \bar{u}(t, x) = u_a \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \geq 0, \\ \bar{u}(t, x) = u_b \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \leq 0, \\ \bar{u}(t, x) \in (u_a, u_b) \Rightarrow \bar{\varphi}(t, x) + \mu \bar{u}(t, x) = 0, \end{cases} \quad (\text{D.21})$$

και

$$\begin{cases} \bar{\varphi}(t, x) + \mu \bar{u}(t, x) > 0 \Rightarrow \bar{u}(t, x) = u_a, \\ \bar{\varphi}(t, x) + \mu \bar{u}(t, x) < 0 \Rightarrow \bar{u}(t, x) = u_b. \end{cases} \quad (\text{D.22})$$

Εισάγουμε τον κώνο των κρίσματων κατευθύνσεων που είναι απαραίτητος για τη διατύπωση των συνθηκών δεύτερης τάξης.

$$\mathcal{C}_{\bar{u}} = \{v \in L_2(0, T; L_2(\Omega)) : v \text{ ικανοποιεί (D.24)}\}, \quad (\text{D.23})$$

$$\begin{cases} i) \quad v(t, x) = 0 \quad \text{αν } \bar{\varphi}(t, x) + \mu \bar{u}(t, x) \neq 0 \\ ii) \quad v(t, x) \geq 0 \quad \text{αν } \bar{u}(t, x) = u_a \\ iii) \quad v(t, x) \leq 0 \quad \text{αν } \bar{u}(t, x) = u_b. \end{cases} \quad (\text{D.24})$$

Παρατηρούμε ότι

$$\begin{aligned} J'(\bar{u})v &= \int_0^T \int_{\Omega} (\bar{\varphi}(t, x) + \mu \bar{u}(t, x)) v(t, x) \, dx \, dt, \\ &(\bar{\varphi}(t, x) + \mu \bar{u}(t, x)) v(t, x) = 0 \text{ για } \sigma.\pi. (t, x) \in \Omega_T \text{ και } \forall v \in \mathcal{C}_{\bar{u}}. \end{aligned} \quad (\text{D.25})$$

Θεώρημα D.9. Έστω \bar{u} μια τοπική λύση του προβλήματος (D.3). Τότε, ισχύει ότι

$$J''(\bar{u})v^2 \geq 0 \quad \forall v \in \mathcal{C}_{\bar{u}}. \quad (\text{D.26})$$

Τώρα, θα αναφέρουμε τις ικανές συνθήκες βελτιστοποίησης.

Θεώρημα D.10. Υποθέτουμε ότι $\bar{u} \in U_{ad}$ ικανοποιεί

$$J'(\bar{u})(u - \bar{u}) \geq 0 \quad \forall u \in U_{ad}, \quad (\text{D.27})$$

$$J''(\bar{u})v^2 > 0 \quad \forall v \in \mathcal{C}_{\bar{u}} \setminus \{0\}, \quad (\text{D.28})$$

τότε υπάρχουν $\alpha > 0$ και $\delta > 0$ τέτοια ώστε

$$J(\bar{u}) + \frac{\delta}{2} \|u - \bar{u}\|_{L_2(0, T; L_2(\Omega))}^2 \leq J(u) \quad \forall u \in U_{ad} \cap B_{\alpha}(\bar{u}), \quad (\text{D.29})$$

όπου $B_{\alpha}(\bar{u})$ είναι η ανοιχτή μπάλα στον $L_2(0, T; L_2(\Omega))$ με κέντρο \bar{u} και ακτίνα α .

Η ικανή συνθήκη δεύτερης τάξης (D.28) είναι ισοδύναμη με

$$J''(\bar{u})v^2 \geq \delta \|v\|_{L_2(0, T; L_2(\Omega))}^2 \quad \forall v \in \mathcal{C}_{\bar{u}}. \quad (\text{D.30})$$

E Κεφάλαιο 6

Παρουσιάζουμε μια εκτίμηση σφάλματος για ένα πλήρως διακριτό σχήμα που βασίζεται στην ασυνεχή -στο χρόνο- μέθοδο Galerkin dG(0), (προσεγγίσεις με κατά τμήματα σταθερές προσεγγίσεις στο χρόνο, πεπερασμένα στοιχεία που βασίζονται σε προσεγγίσεις με κατά τμήματα γραμμικά πολυώνυμα στο χώρο). Η αριθμητική ανάλυση του ελέγχου προς την κατάσταση με υποθέσεις χαμηλής ομαλότητας βασίζεται σε κρίσιμη τροποποίηση της προσέγγισης των [BMO11, BM11] που είναι η ορισμός μιας ολικά χωροχρονικής προβολής ως η $dG(0)$ λύση μιας εξίσωσης θερμότητας με δεξιά μέλος $y_t - \Delta y$ (παρόμοια με προηγούμενες εργασίες των [CW10] (μη ελεγχόμενες εξισώσεις Navier-Stokes), [CC12] (για τις ελεγχόμενες Navier-Stokes) και [Chr19] (για τις μη ελεγχόμενες Allen-Cahn)). Στην προσέγγισή μας δεν υποθέτουμε κανένα σημειακό χωροχρονικό άνω φράγμα της πλήρως διακριτής λύσης της απεικόνισης του ελέγχου στην κατάσταση και το πιο κρίσιμο είναι ότι δεν κατασκευάζουμε μια διακριτή προσέγγιση της φασματικής εκτίμησης, με αποτέλεσμα η εκτίμηση να είναι έγκυρη υπό περιορισμένες υποθέσεις ομαλότητας που επιβάλλονται στο πλαίσιο του βέλτιστου ελέγχου. Για την αριθμητική ανάλυση της διακριτής απεικόνισης συζύγους κατάστασης, η βασική δυσκολία είναι η ανάπτυξη διακριτών εκτιμήσεων ευστάθειας και σφάλματος που εξαρτώνται πολυωνυμικά από το $1/\epsilon$. Πράγματι, σημειώνουμε ότι η φασματική εκτίμηση δεν ισχύει πλέον αν αντικαταστήσουμε το y με τη διακριτοποίησή του και η άμεση εφαρμογή του μη γραμμικού Λήμματος Gronwall θα οδηγήσει σε σοβαρούς περιορισμούς στο μέγεθος του $\|y_u - y_d\|_{L_2(0,T;L_2(\Omega))}$ και $\|y(T) - y_\Omega\|_{L_2(\Omega)}$ σε όρους ϵ που δεν είναι κατάλληλοι στο πλαίσιο του βέλτιστου ελέγχου. Η προσέγγισή μας βασίζεται σε ένα ψευδοδυϊκό επιχείρημα που αποφεύγει την κατασκευή μιας διακριτής προσέγγισης της φασματικής εκτίμησης και τη χρήση ενός μη γραμμικού Λήμματος Gronwall και οδηγεί σε διακριτές εκτιμήσεις ευστάθειας. Στη συνέχεια, στην απόδειξη εκτιμήσεων σφάλματος για τη διακριτή απεικόνιση της κατάστασης προς την συζυγή κατάσταση, χρησιμοποιούμε ένα επιχείρημα *boot-strap*. Σημειώνουμε ότι η ανάλυση σφάλματος της απεικόνισης κατάστασης προς τη συζυγή κατάσταση είναι ανεξάρτητη του ενδιαφέροντος, καθώς αφορά ένα γραμμικό πρόβλημα με χαμηλής ομαλότητας υποθέσεις στα δεδομένα. Συνδυάζοντας αυτές τις εκτιμήσεις, είμαστε σε θέση να προχωρήσουμε παρόμοια με το [CC12] να αποδείξουμε επιθυμητές εκτιμήσεις για τη διαφορά μεταξύ των τοπικών βέλτιστων ελέγχων και της διακριτής προσέγγισής τους, καθώς και εκτιμήσεις για τις διαφορές μεταξύ της αντίστοιχης κατάστασης και της συζυγούς κατάστασης και των διακριτών προσεγγίσεών τους.

E.1 Διακριτοποίηση

Έστω $\{\mathcal{T}_h\}_{h>0}$ μια οικογένεια τριγωνοποιήσεων του $\bar{\Omega}$. Θεωρούμε ότι κάθε \mathcal{T}_h είναι σύμορφη και σχηματικά ομαλή υποδιαίρεση τέτοια ώστε $\cup_{\tau \in \mathcal{T}_h} \tau = \bar{\Omega}$. Σε κάθε στοιχείο $\tau \in \mathcal{T}_h$ αντιστοιχίζουμε δύο παραμέτρους h_τ και ρ_τ , όπου h_τ η διάμετρος του τ ενώ ρ_τ η διάμετρος της μεγαλύτερης μπάλας που περιέχεται στο τ . Στη συνέχεια, ορίζουμε την παράμετρο διακριτοποίησης του πλέγματος ως $h := \max_{\tau \in \mathcal{T}_h} h_\tau$. Σε κάθε \mathcal{T}_h αντιστοιχεί ο χώρος πεπερασμένων στοιχείων:

$$Y_h := \{y_h \in C(\bar{\Omega}); y_h|_\tau \in \mathbb{P}_1(\tau), \quad \forall \tau \in \mathcal{T}_h\} \subset H_0^1(\Omega),$$

\mathbb{P}_1 , ο d -μεταβλητός χώρος των γραμμικών πολυωνύμων. Επιπλέον, ορίζουμε

$$U_h = \{u_h \in L_2(0, T; L_2(\Omega)); u_h|_{\tau} \equiv u_{\tau} \in \mathbb{R}\}.$$

Έστω $0 = t_0 < t_1 < \dots < t_N = T$. Διαμερίζουμε το $[0, T]$ σε υποδιαστήματα $J_n := (t_{n-1}, t_n]$ με $k_n := t_n - t_{n-1}$, $n = 1, \dots, N$ το χρονικό βήμα. Υποθέτουμε ότι

$$\exists C_0 > 0 \text{ τ.ω. } k = \max_{1 \leq n \leq N} k_n < C_0 k_n \quad \forall 1 \leq n \leq N \text{ και } \forall k > 0. \quad (\text{E.1})$$

Θέτουμε $\sigma = (k, h)$ και θεωρούμε τους ακόλουθους πλήρως διακριτούς χώρους:

$$\begin{aligned} Y_{\sigma} &:= \{y_{\sigma} \in L_2(0, T; H_0^1(\Omega)); y_{\sigma}|_{J_n} \in Y_h, 1 \leq n \leq N\}, \\ U_{\sigma} &:= \{u_{\sigma} \in L_2(0, T; L_2(\Omega)); u_{\sigma}|_{J_n} \in U_h, 1 \leq n \leq N\}. \end{aligned}$$

Οι συναρτήσεις των Y_{σ} και U_{σ} είναι κατά τημήματα σταθερές στο χρόνο. Ψάχνουμε για διακριτούς ελέγχους στο U_{σ} στη μορφή:

$$u_{\sigma} = \sum_{n=1}^N \sum_{\tau \in \mathcal{T}_h} u_{n,\tau} \chi_n \chi_{\tau}, \quad \text{με } u_{n,\tau} \in \mathbb{R},$$

χ_n, χ_{τ} είναι οι χαρακτηριστικές συναρτήσεις επί (t_{n-1}, t_n) και τ , αντίστοιχα. Θεωρούμε το κυρτό υποσύνολο του U_{σ} ,

$$U_{\sigma,ad} = U_{\sigma} \cap U_{ad} = \{u_{\sigma} \in U_{\sigma} : u_{n,\tau} \in [u_a, u_b]\}.$$

Κάθε στοιχείο του Y_{σ} γράφεται ως

$$y_{\sigma} = \sum_{n=1}^N y_{n,h} \chi_n, \quad \text{με } y_{n,h} \in Y_h.$$

Θέτουμε $y_{\sigma}(t_n) = y_{n,h}$ προκειμένου το y_{σ} να είναι συνεχές από αριστερά. Έτσι, έχουμε $y_{\sigma}(T) = y_{\sigma}(t_N) = y_{N,h}$. Για να εισαγάγουμε το διακριτό πρόβλημα ελέγχου, πρέπει να ορίσουμε το πλήρως διακριτό σχήμα της εξίσωσης κατάστασης (D.2). Για κάθε $u \in L_2(0, T; L_2(\Omega))$, για κάθε $n = 1, \dots, N$ και για όλα $w_h \in Y_h$,

$$\left(\frac{y_{n,h} - y_{n-1,h}}{k_n}, w_h \right) + (\nabla y_{n,h}, \nabla w_h) + \epsilon^{-2} (F(y_{n,h}), w_h) = (u_n, w_h) \quad (\text{E.2})$$

$$y_{0,h} = y_{0h},$$

όπου

$$u_n = \frac{1}{k_n} \int_{t_{n-1}}^{t_n} u(t) dt, \quad (\text{E.3})$$

$$y_{0h} \in Y_h \quad \text{τ.ω. } \|y_0 - y_{0h}\|_{L_2(\Omega)} \leq Ch \quad \text{και } \|y_{0h}\|_{H^1(\Omega)} \leq C \quad \forall h > 0.$$

Ορίζουμε το διακριτό πρόβλημα ελέγχου ως εξής,

$$\left\{ \begin{array}{l} \min J_{\sigma}(u_{\sigma}) \\ u_{\sigma} \in U_{\sigma,ad}, \end{array} \right. \quad (\text{E.4})$$

όπου

$$\begin{aligned} J_\sigma(u_\sigma) = & \frac{1}{2} \int_0^T \int_\Omega |y_\sigma(u_\sigma) - y_d(t, x)|^2 dx dt + \frac{\gamma}{2} \int_\Omega |y_\sigma(T) - y_{\Omega,h}|^2 dx \\ & + \frac{\mu}{2} \int_0^T \int_\Omega |u_\sigma|^2 dx dt, \end{aligned} \quad (\text{E.5})$$

$$y_{\Omega,h} \in Y_h \text{ τ.ω. } \|y_\Omega - y_{\Omega,h}\|_{L_2(\Omega)} \leq Ch \text{ και } \|y_{\Omega,h}\|_{H^1(\Omega)} \leq C \forall h > 0. \quad (\text{E.6})$$

E.2 Ανάλυση της διακριτής εξίσωσης κατάστασης

Έστω $y = y_u = G(u)$ και $y_\sigma = y_\sigma(u) \in Y_\sigma$ λύση του (E.4). Αρχικά παρουσιάζουμε κάποιες διακριτές εκτιμήσεις ευστάθειας που είναι χρήσιμες για την επικείμενη ανάλυση.

Ορισμός E.1. Ορίζουμε τον τελεστή προβολής $P_h : L_2(\Omega) \rightarrow Y_h$, $(P_h y, w_h) = (y, w_h) \quad \forall w_h \in Y_h$. Επίσης, ορίζουμε $P_\sigma : C(0, T; L_2(\Omega)) \rightarrow Y_\sigma$ όπου $(P_\sigma y)_{n,h} = P_h y(t_n)$, για κάθε $1 \leq n \leq N$.

Λήμμα E.2. Έστω y_σ λύση της (E.4) που αντιστοιχεί στη συνάρτηση ελέγχου $u \in L_2(0, T; L_2(\Omega))$ και $y_{0h} := P_h y_0$. Τότε, υπάρχει σταθερά $C > 0$ ανεξάρτητη των $\sigma = (k, h), \epsilon$ και $\|y\|_{L_\infty(0, T; L_\infty(\Omega))}$, τέτοια ώστε

$$\begin{aligned} & \|y_\sigma\|_{L_2(0, T; L_2(\Omega))} + \|y_\sigma\|_{L_4(0, T; L_4(\Omega))}^2 \\ & \leq C(|\Omega_T|^{\frac{1}{2}} + \|y_0\|_{L_2(\Omega)} + \|u\|_{L_2(0, T; L_2(\Omega))}) := C_{st,1}^{\text{dG}}, \end{aligned}$$

and

$$\begin{aligned} & \|y_\sigma\|_{L_\infty(0, T; L_2(\Omega))} + \|y_\sigma\|_{L_2(0, T; H^1(\Omega))} \\ & + \left(\sum_{n=1}^N \|y_{n,h} - y_{n-1,h}\|_{L_2(\Omega)}^2 \right)^{1/2} \leq \frac{C_{st,1}^{\text{dG}}}{\epsilon}. \end{aligned}$$

Αν επιπλέον, $k \leq \frac{3C_0\epsilon^2}{2}$, με C_0 όπως στην (E.1), τότε ισχύει η ακόλουθη εκτίμηση,

$$\begin{aligned} & \|y_\sigma\|_{L_\infty(0, T; H_0^1(\Omega))} + \frac{1}{\epsilon} \|y_\sigma\|_{L_\infty(0, T; L_4(\Omega))}^2 \\ & \leq C \left(\|\nabla y_{0h}\|_{L_2(\Omega)} + \frac{1}{\epsilon} \|y_{0h}\|_{L_4(\Omega)}^2 + \frac{|\Omega|^{1/2}}{\epsilon} + \|u\|_{L_2(0, T; L_2(\Omega))} \right) := C_{st,2}^{dG}. \end{aligned}$$

Λήμμα E.3. Υπάρχει σταθερά $C > 0$ ανεξάρτητη του σ τέτοια ώστε για κάθε $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ να ισχύει ότι

$$\begin{aligned} \|y - P_\sigma y\|_{L_2(0, T; L_2(\Omega))} & \leq C \left(k \|y_t\|_{L_2(0, T; L_2(\Omega))} + h^2 \|y\|_{L_2(0, T; H^2(\Omega))} \right), \\ \|y - P_\sigma y\|_{L_2(0, T; H_0^1(\Omega))} & \leq C \left(\sqrt{k} \|y_t\|_{L_2(0, T; L_2(\Omega))} + (\sqrt{k} + h) \|y\|_{L_2(0, T; H^2(\Omega))} \right). \end{aligned}$$

Ένα άλλο τεχνικό εργαλείο είναι ο ορισμός μιας χωροχρονικής προβολής στον Y_σ ως μια διακριτή λύση του βοηθητικού γραμμικού παραβολικού προβλήματος. Έστω $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ η λύση του (D.2) και $y_{0h} := P_h y_0$. Ορίζουμε ότι $\hat{y}_\sigma \in Y_\sigma$ να ικανοποιεί: Για κάθε $n = 1, \dots, N$ και $\forall w_h \in Y_h$

$$\left(\frac{\hat{y}_{n,h} - \hat{y}_{n-1,h}}{k_n}, w_h \right) + (\nabla \hat{y}_{n,h}, \nabla w_h) = (\hat{f}_n, w_h), \quad (\text{E.7})$$

$$\hat{y}_{0,h} = y_{0h},$$

όπου

$$\begin{aligned} (\hat{f}_n, w_h) &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \{(\nabla y(t), \nabla w_h) + (y_t(t), w_h)\} dt \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (\nabla y(t), \nabla w_h) dt + \left(\frac{y(t_n) - y(t_{n-1})}{k_n}, w_h \right). \end{aligned}$$

Λήμμα E.4. Ας υποθέσουμε ότι $\hat{y}_\sigma \in Y_\sigma$ είναι η λύση της (E.7). Τότε, υπάρχει $C > 0$ ανεξάρτητη από το σ τέτοια ώστε,

$$\begin{aligned} \|y - \hat{y}_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \|y - \hat{y}_\sigma\|_{L_2(0,T;H_0^1(\Omega))} &\leq C(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}, \\ \|y - \hat{y}_\sigma\|_{L_2(0,T;L_2(\Omega))} &\leq C(k+h^2)\|y\|_{H^{2,1}(\Omega_T)}. \end{aligned}$$

Το ακόλουθο αποτέλεσμα αποτελεί την κύρια εκτίμηση σφάλματος για την απεικόνιση ελέγχου προς κατάσταση. Τονίζουμε ότι, σε αντίθεση με προηγούμενες εργασίες για την μη ελεγχόμενη εξίσωση Allen-Cahn, δεν υπερβαίνουμε την ομαλότητα $H^{2,1}(\Omega_T)$. Η τεχνική μας αξιοποιεί τη φασματική εκτίμηση σε “συνεχές επίπεδο”, και κατά συνέπεια αποφεύγουμε την κατασκευή διακριτών προσεγγίσεων, οι οποίες συνήθως οδηγούν σε υποθέσεις περισσότερης ομαλότητας.

Θεώρημα E.5. Εστω $u \in L_2(0, T; L_2(\Omega))$, $y \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ και $y_\sigma \in Y_\sigma$ ικανοποιούν (D.2) και (E.2) αντίστοιχα. Υποθέτουμε ότι $\|\lambda\|_{L_\infty(0,T)} \leq C$.

1. Για $d = 2$, αν υπάρχει $C > 0$ έτσι ώστε

$$\begin{aligned} &(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}^{1/2} \max\left\{\frac{C_\infty}{\epsilon}, \|y\|_{H^{2,1}(\Omega_T)}\right\}^{1/2} \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{1/2} \\ &\leq \epsilon^2 CE^{-1/2}, \end{aligned} \quad (\text{E.8})$$

τότε ισχύουν οι ακόλουθες εκτιμήσεις:

$$\begin{aligned} &\|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1}\|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ &\leq \max\left\{\frac{C_I}{\epsilon^2}(\sqrt{k}+h), \frac{C_{II}}{\epsilon}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}, C\right\}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}, \end{aligned} \quad (\text{E.9})$$

$$\begin{aligned} &\|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \\ &\leq \max\left\{\frac{C_I}{\epsilon^3}(\sqrt{k}+h), \frac{C_{II}}{\epsilon^2}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}, C\right\}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}. \end{aligned} \quad (\text{E.10})$$

2. Για $d = 3$, αν υπάρχει $C > 0$ έτσι ώστε

$$(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}^{4/3}\|y\|_{L_\infty(0,T;L_\infty(\Omega))}^{2/3} \leq \epsilon^3 CE^{-1}, \quad (\text{E.11})$$

τότε ισχύουν οι ακόλουθες εκτιμήσεις:

$$\begin{aligned} &\|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1}\|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 \\ &\leq \max\left\{\frac{C_{II}}{\epsilon}(\sqrt{k}+h)^{1/2}\|y\|_{H^{2,1}(\Omega_T)}, C\right\}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}, \end{aligned} \quad (\text{E.12})$$

$$\begin{aligned} &\|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \\ &\leq \max\left\{\frac{C_{II}}{\epsilon^2}(\sqrt{k}+h)^{1/2}\|y\|_{H^{2,1}(\Omega_T)}, C\right\}(\sqrt{k}+h)\|y\|_{H^{2,1}(\Omega_T)}. \end{aligned} \quad (\text{E.13})$$

Εδώ, συμβολίζουμε με $C_I := 2E^{1/2}C_\infty$, $C_{II} := CE^{1/2}$ και $E := \exp(2T\alpha)$ όπου

$$C_\infty := C \left(1 + (1 + \epsilon^2) \|y\|_{L_\infty(0,T;L_\infty(\Omega))}^2 \right)^{1/2}, \quad \alpha := \sup_{t \in [0,T]} (2\lambda(t)(1 - \epsilon^2) + 4),$$

$C > 0$, αλγεβρική σταθερά (που μπορεί να είναι διαφορετική σε κάθε περίπτωση) αλλά ανεξάρτητη από σ, ϵ , και $\|y\|_{L_\infty(0,T;L_\infty(\Omega))}$.

Ανακαλούμε ότι $C_I \sim \|y\|_{L_\infty(0,T;L_\infty(\Omega))}$ και $\|y\|_{H^{2,1}(\Omega_T)} \sim \epsilon^{-r}$, $r \in \{1, 2\}$. Υποθέτουμε ότι υπάρχει σταθερά $C > 0$ ανεξάρτητη των σ, ϵ τέτοια ώστε: $\|y\|_{L_\infty(0,T;L_\infty(\Omega))} \leq C$. Θα προσδιορίσουμε τον κυρίαρχο όρο στις εκτιμήσεις του Θεωρήματος E.5. Πράγματι, για $d = 2$ το (E.8) γίνεται

$$(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)} \leq C \epsilon^2 \implies \sqrt{k} + h \leq C \epsilon^{2+r}, \quad (\text{E.14})$$

όπου C , αλγεβρική σταθερά που εξαρτάται μόνο από το χωρίο και $\|\lambda\|_{L_\infty(0,T)}$, και συνεπώς αντικαθιστώντας (E.14) στις εκτιμήσεις (E.9) και (E.10) έχουμε

$$\begin{aligned} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 &\leq C(\sqrt{k} + h) \epsilon^{-r}, \\ \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} &\leq C(\sqrt{k} + h) \epsilon^{-r}. \end{aligned}$$

Για $d = 3$, συμπεραίνουμε ότι η (E.11) γίνεται

$$(\sqrt{k} + h) \|y\|_{H^{2,1}(\Omega_T)}^{4/3} \leq C \epsilon^3 \implies \sqrt{k} + h \leq C \epsilon^{3+(4r/3)}, \quad (\text{E.15})$$

και οι (E.12) και (E.13) γράφονται ως εξής:

$$\begin{aligned} \|y - y_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon^{-1} \|y - y_\sigma\|_{L_4(0,T;L_4(\Omega))}^2 &\leq C(\sqrt{k} + h) \epsilon^{-(7r-1)/6}, \\ \|y - y_\sigma\|_{L_2(0,T;H_0^1(\Omega))} &\leq C(\sqrt{k} + h) \epsilon^{-(8r+3)/6}. \end{aligned}$$

Πόρισμα E.6. Έστω $u, v \in L_2(0, T; L_2(\Omega))$, $y_u \in H^{2,1}(\Omega_T) \cap C(0, T, H_0^1(\Omega))$ η λύση της (D.2) ενώ $y_\sigma(v) \in Y_\sigma$ η λύση της (E.2) που αντιστοιχεί στον έλεγχο v . Υποθέτουμε ότι ισχύουν οι υποθέσεις των άτων D.3 και E.5. Επιπλέον, έστω $\|y_v\|_{L_\infty(0,T;L_\infty(\Omega))} \leq C$, και $\|y_v\|_{H^{2,1}(\Omega_T)} \leq C \epsilon^{-r}$ με $r \in \{1, 2\}$, όπου C σταθερά που εξαρτάται μόνο από τα δεδομένα και είναι ανεξάρτητη του ϵ και ότι (E.14) ή (E.15) ισχύουν για $d = 2$ ή 3 , αντίστοιχα. Τότε, για $d = 2$

$$\|y_u - y_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} \leq L_1 \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^r} (\sqrt{k} + h), \quad (\text{E.16})$$

$$\|y_u - y_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{L_1}{\epsilon} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^r} (\sqrt{k} + h), \quad (\text{E.17})$$

ενώ για $d = 3$, έχουμε

$$\|y_u - y_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} \leq L_1 \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^{(7r-1)/6}} (\sqrt{k} + h), \quad (\text{E.18})$$

$$\|y_u - y_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{L_1}{\epsilon} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{C}{\epsilon^{(8r+3)/6}} (\sqrt{k} + h). \quad (\text{E.19})$$

Έστω $u_\sigma \in U_\sigma$. Αν $u_\sigma \rightarrow u$ ασθενώς στο $L_2(0, T; L_2(\Omega))$ για κάθε σ , τότε

$$\begin{cases} \|y_u - y_\sigma(u_\sigma)\|_{L_2(0,T;H_0^1(\Omega))} \rightarrow 0, \\ \|y_u - y_\sigma(u_\sigma)\|_{L_p(0,T;L_2(\Omega))} \rightarrow 0 \quad \forall 1 \leq p < \infty, \\ \|y_u(T) - y_\sigma(u_\sigma)(T)\|_{L_2(\Omega)} \rightarrow 0. \end{cases} \quad (\text{E.20})$$

Το επόμενο θεώρημα μελετά τη παραγωγισμότητα της σχέσης ελέγχου και διακριτής κατάστασης.

Θεώρημα E.7. Έστω $u, v \in L_2(0, T; L_2(\Omega))$. Η απεικόνιση $G_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow Y_\sigma$, ώστε $y_\sigma = y_\sigma(u) = G_\sigma(u)$, είναι κλάσης C^∞ . Συμβολίζουμε με $z_\sigma(v) = G'_\sigma(u)v$ τη μοναδική λύση του προβλήματος: Για $n = 1, \dots, N$ και για κάθε $w_h \in Y_h$,

$$\begin{aligned} & \left(\frac{z_{n,h} - z_{n-1,h}}{k_n}, w_h \right) + (\nabla z_{n,h}, \nabla w_h) + \epsilon^{-2} ((3y_{n,h}^2 - 1)z_{n,h}, w_h) \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (v(t), w_h) dt, \quad \text{with } z_{0,h} = 0. \end{aligned} \quad (\text{E.21})$$

E.3 Ανάλυση της διακριτής εξίσωσης συζυγούς κατάστασης

Οι ιδιότητες παραγωγισμότητα του $G_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow Y_\sigma$ συνεπάγονται ότι η συνάρτηση κόστους $J'_\sigma : L_2(0, T; L_2(\Omega)) \rightarrow \mathbb{R}$ είναι επίσης C^∞ . Εφαρμόζοντας τον κανόνα της αλυσίδας, έχουμε

$$\begin{aligned} J'_\sigma(u)v &= \int_0^T \int_\Omega (y_\sigma - y_d) z_\sigma dx dt + \gamma \int_\Omega (y_\sigma(T) - y_{\Omega,h}) z_\sigma(T) dx \\ &\quad + \mu \int_0^T \int_\Omega uv dx dt, \end{aligned} \quad (\text{E.22})$$

Θεωρούμε το αντίστοιχο διακριτό σχήμα της εξίσωσης συζυγούς κατάστασης (D.11): Για κάθε $n = N, \dots, 1$ και για όλα τα $w_h \in Y_h$,

$$\begin{aligned} & \left(\frac{\varphi_{n,h} - \varphi_{n+1,h}}{k_n}, w_h \right) + (\nabla \varphi_{n,h}, \nabla w_h) + \epsilon^{-2} ((3y_{n,h}^2 - 1)\varphi_{n,h}, w_h) \\ &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} (y_{n,h} - y_d(t), w_h) dt, \\ & \varphi_{N+1,h} = \gamma (y_{N,h} - y_{\Omega,h}). \end{aligned} \quad (\text{E.23})$$

Τότε, η (E.22) μπορεί να γραφτεί ως εξής

$$J'_\sigma(u)v = \int_0^T \int_\Omega (\varphi_\sigma + \mu u) v dx dt, \quad \forall v \in L_2(0, T; L_2(\Omega)). \quad (\text{E.24})$$

Το ακόλουθο Λήμμα περιλαμβάνει βασικές εκτιμήσεις ευστάθειας του (E.23).

Λήμμα E.8. Έστω $u \in L_2(0, T; L_2(\Omega))$, $y_u \in H^{2,1}(\Omega_T) \cap C(0, T; H_0^1(\Omega))$ λύση της (D.2) ενώ $y_\sigma(u) \equiv y_\sigma \in Y_\sigma$ λύση της (E.2) που αντιστοιχεί στον έλεγχο u . Υποθέτουμε ότι ισχύουν οι υποθέσεις του Θεωρήματος D.3. Έστω $C_\infty \sim \|y_u\|_{L_\infty(0,T;L_\infty(\Omega))}$, and $\|y_u\|_{H^{2,1}(\Omega_T)} \leq C\epsilon^{-r}$ με $r \in \{1, 2\}$, όπου C σταθερά που εξαρτάται μόνο από τα δεδομένα και είναι ανεξάρτητη από το ϵ και $C_\zeta := \exp \left(\int_0^T 2\lambda(t)(1-\epsilon^2) + 3 dt \right)$, και ότι (E.14) ή (E.15) ισχύουν για $d = 2$ ή 3 , αντίστοιχα. Εάν επιπλέον,

$$\begin{aligned} \sqrt{k} + h &\leq \frac{C\epsilon^{2+r}}{C_\infty C_\zeta} \quad \text{για } d = 2, \\ \sqrt{k} + h &\leq \frac{C\epsilon^{3+(4r/3)}}{C_\infty C_\zeta} \quad \text{για } d = 3, \end{aligned} \quad (\text{E.25})$$

υπάρχει $D_{st,1}^{dG} > 0$ (ανεξάρτητη των $\sigma = (k, h)$ και ϵ) έτσι ώστε:

$$\|\nabla \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))} + \epsilon^{-1} \|y_\sigma \varphi_\sigma\|_{L_2(0,T;L_2(\Omega))} \leq \frac{D_{st,1}^{dG}}{\epsilon}.$$

Εδώ, $D_{st,1}^{dG} := C (\gamma \|y_{N,h} - y_{\Omega,h}\|_{L_2(\Omega)} + \|y_\sigma - y_d\|_{L_2(0,T;L_2(\Omega))})$ με C αλγεβρική σταθερά ανεξάρτητη από ϵ .

Θεώρημα E.9. Έστω $u \in L_2(0, T; L_2(\Omega))$ και $y, \varphi \in H^{2,1}(\Omega_T) \cap C(0, T, H_0^1(\Omega))$ είναι η λύση της κατάστασης (D.2) και η λύση της συζυγούς κατάστασης (D.11), αντίστοιχα. Έστω, y_σ η διακριτή λύση κατάστασης του (E.2) ενώ φ_σ η διακριτή λύση συζυγούς κατάστασης του (E.23). Τότε, υπό τις υποθέσεις του Θεωρήματος E.5 και του Λήμματος E.8 υπάρχει $\hat{C} > 0$ τέτοια ώστε για $r \in \{1, 2\}$ να ισχύει ότι:

$$\|\varphi - \varphi_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi - \varphi_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{4+r}} \quad \text{για } d = 2, \quad (\text{E.26})$$

$$\|\varphi - \varphi_\sigma\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi - \varphi_\sigma\|_{L_2(0,T;H_0^1(\Omega))} \leq \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{4+(7r-1)/6}} \quad \text{για } d = 3; \quad (\text{E.27})$$

με $E := \exp(T\alpha)$ όπου $\alpha := \sup_{t \in [0, T]} (2\lambda(t)(1 - \epsilon^2) + 5)$ και
 $\hat{C} := C(E^{1/2} (C_{st,2}^{dG} + C_{st,2}) D_{st,1}^{dG})$.

Το ακόλουθο αποτέλεσμα είναι ανάλογο με το Πόρισμα E.6 και άμεση συνέπεια του Θεωρήματος E.9 και του Λήμματος D.7

Πόρισμα E.10. Έστω $u, v \in L_2(0, T; L_2(\Omega))$ και $\varphi_u \in H^{2,1}(\Omega_T) \cap C(0, T, H_0^1(\Omega))$ η λύση της (5.16) ενώ $\varphi_\sigma(v) \in Y_\sigma$ η λύση της (E.23) που αντιστοιχεί στον έλεγχο v . Έστω ότι ισχύουν τα Λήμματα D.7 και E.8 και το Θεώρημα E.9 και έστω $r \in \{1, 2\}$. Τότε, για $d = 2$ ισχύει

$$\begin{aligned} & \|\varphi_u - \varphi_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi_u - \varphi_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \frac{L_2}{\epsilon^{7/2}} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{4+r}}, \end{aligned} \quad (\text{E.28})$$

ενώ για $d = 3$ προκύπτει ότι

$$\begin{aligned} & \|\varphi_u - \varphi_\sigma(v)\|_{L_\infty(0,T;L_2(\Omega))} + \epsilon \|\varphi_u - \varphi_\sigma(v)\|_{L_2(0,T;H_0^1(\Omega))} \\ & \leq \frac{L_3}{\epsilon^{15/4}} \|u - v\|_{L_2(0,T;L_2(\Omega))} + \frac{\hat{C}(\sqrt{k} + h)}{\epsilon^{4+(7r-1)/6}}. \end{aligned} \quad (\text{E.29})$$

Σύμφωνα με τον συμβολισμό του λήμματος D.7 έχουμε

$$\begin{aligned} L_2 &:= L_1 \left(\epsilon^{7/2} C_T E_\varphi^{1/2} + \tilde{c} C_\infty^{1/2} D_{st,1} \right), \\ L_3 &:= L_1 \left(\epsilon^{15/4} C_T E_\varphi^{1/2} + \tilde{c} C_\infty^{1/2} D_{st,1} \right). \end{aligned}$$

E.4 Σύγκλιση του διακριτού προβλήματος ελέγχου

Μελετάμε τη σύγκλιση των λύσεων του διακριτού προβλήματος ελέγχου (E.4) προς τις λύσεις του συνεχούς προβλήματος (5.45). Κάθε διακριτό πρόβλημα (E.4) έχει τουλάχιστον μία λύση επειδή η συνάρτηση ελαχιστοποίησης είναι συνεχής και πιεστική σε ένα μη κενό κλειστό υποσύνολο ενός χώρου πεπερασμένης διάστασης.

Θεώρημα E.11. Για κάθε $\sigma = (k, h)$, έστω \bar{u}_σ μια ολική λύση του προβλήματος (E.4). Τότε, η ακολουθία $\{\bar{u}_\sigma\}_\sigma$ είναι φραγμένη στον $L_2(0, T; L_2(\Omega))$ και υπάρχουν υποακολουθίες που συμβολίζονται με τον ίδιο τρόπο και συγκλίνουν σε ένα σημείο \bar{u} ασθενώς στον $L_2(0, T; L_2(\Omega))$. Οποιοδήποτε από αυτά τα οριακά σημεία αποτελεί λύση του προβλήματος (E.4). Επιπλέον, έχουμε

$$\lim_{\sigma \rightarrow 0} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0, T; L_2(\Omega))} = 0 \quad \text{and} \quad \lim_{\sigma \rightarrow 0} J_\sigma(\bar{u}_\sigma) = J(\bar{u}). \quad (\text{E.30})$$

Θεώρημα E.12. Έστω \bar{u} ένα αυστηρό τοπικό ελάχιστο του (5.45). Τότε, υπάρχει μια ακολουθία $\{\bar{u}_\sigma\}_\sigma$ τοπικών ελαχίστων των προβλημάτων (E.4) τέτοια ώστε να ισχύει η (E.30).

Συμβολίζουμε με \bar{u} μια τοπική λύση της (5.45) και \bar{u}_σ μια τοπική λύση της (E.4) για κάθε σ . Από τα Θεωρήματα E.11 - E.12, συμπεραίνουμε ότι $\|\bar{u} - \bar{u}_\sigma\|_{L_2(0, T; L_2(\Omega))} \rightarrow 0$. Επιπλέον, έστω \bar{y} και $\bar{\varphi}$ η κατάσταση και η συζυγής κατάσταση που αντιστοιχούν στο \bar{u} ενώ \bar{y}_σ και $\bar{\varphi}_\sigma$ η διακριτή κατάσταση και η διακριτή συζυγής κατάσταση που αντιστοιχούν στο \bar{u}_σ .

Θεώρημα E.13. Ας υποθέσουμε ότι οι υποθέσεις των Θεωρημάτων D.8 και D.10 και των Πορισμάτων E.6 και E.10 ισχύουν. Τότε, υπάρχουν $\mathcal{C} := \sqrt{T}\hat{C}$, $\tilde{\mathcal{C}} := L_1\mathcal{C}$ τέτοιες ώστε για $d = 2$ και $r = 1, 2$,

$$\begin{aligned} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0, T; L_2(\Omega))} &\leq \frac{\mathcal{C}}{\epsilon^{5+r}}(\sqrt{k} + h), \\ \|\bar{y} - \bar{y}_\sigma\|_{L_\infty(0, T; L_2(\Omega))} + \epsilon \|\bar{y} - \bar{y}_\sigma\|_{L_2(0, T; H_0^1(\Omega))} &\leq \frac{\tilde{\mathcal{C}}}{\epsilon^{5+r}}(\sqrt{k} + h). \end{aligned}$$

Επιπλέον, για $d = 3$ και $r = 1, 2$ ισχύουν

$$\begin{aligned} \|\bar{u} - \bar{u}_\sigma\|_{L_2(0, T; L_2(\Omega))} &\leq \frac{\mathcal{C}}{\epsilon^{5+(7r-1)/6}}(\sqrt{k} + h), \\ \|\bar{y} - \bar{y}_\sigma\|_{L_\infty(0, T; L_2(\Omega))} + \epsilon \|\bar{y} - \bar{y}_\sigma\|_{L_2(0, T; H_0^1(\Omega))} &\leq \frac{\tilde{\mathcal{C}}}{\epsilon^{5+(7r-1)/6}}(\sqrt{k} + h). \end{aligned}$$

F Κεφάλαιο 7

Θα συζητήσουμε τώρα ορισμένες πτυχές της περαιτέρω έρευνας που προκύπτουν άμεσα από την εργασία αυτή. Ένα ενδιαφέρον θέμα αποτελεί η χρήση προσαρμοστικών αλγορίθμων για τις εκ των προτέρων εκτιμήσεις σφαλμάτων που αποδείχθηκαν στην πρώτη μας εργασία [CGP20], Κεφάλαιο 3. Το ενδιαφέρον μας να αποδείξουμε εκ των υστέρων εκτιμήσεις σφαλμάτων στην $L_4(0, T; L_4(\Omega))$ -νόρμα είναι, κατά την άποψή μας, δικαιολογημένη, καθώς μπορούν δυνητικά να χρησιμοποιηθούν για την ανάπτυξη χωροχρονικών προσαρμοστικών αλγορίθμων χωρίς υπερβολική αύξηση των βαθμών ελευθερίας. Ως αποτέλεσμα, ο σχεδιασμός τέτοιων αλγορίθμων για την προτεινόμενη ανάδρομη μέθοδο Euler στο χρόνο σε συνδυασμό με σύμμορφη μέθοδο πεπερασμένων στοιχείων στο χώρο θα μπορούσε να αξιολογήσει την πρακτική αξία της ανάλυσης. Επιπλέον, επισημάναμε ότι η νέα εκ των υστέρων ανάλυση σφαλμάτων φαίνεται να βελτιώνει την ϵ -εξάρτηση των συνθηκών (παραδοχών) στις $L_2(0, T, H^1(\Omega))$ - και $L_\infty(0, T; L_2(\Omega))$ -νόρμες σε σύγκριση με προηγούμενες εργασίες των [FW05, Bar05, BMO11, BM11] τουλάχιστον σε ορισμένες περιπτώσεις. Βεβαίως, είναι σαφές ότι η απόδοσή τους πρέπει να αξιολογηθεί αριθμητικά πριν φτάσουμε σε καταληκτικά συμπεράσματα.

Η ανάλυση του Κεφαλαίου 4 ασχολείται με την απόδειξη υπό συνθήκη εκ των υστέρων εκτιμήσεων σφαλμάτος για τις πλήρως διακριτές προσεγγίσεις πεπερασμένων στοιχείων DG-IPDG της εξίσωσης Allen-Cahn σε γενικά πολυτοπικά πλέγματα. Η υλοποίηση των παραπάνω αλγορίθμων αποτελεί από μόνη της ένα ενδιαφέρον και απαιτητικό έργο, το οποίο βρίσκεται υπό προετοιμασία. Πηγαίνοντας ένα βήμα παραπέρα, η αξιοποίηση της μεθόδου DG-IPDG χρησιμοποιώντας πολυωνυμικούς χώρους που ορίζονται σε physical frame, υποδεικνύει τη χρήση υπολογιστικών πλέγματων που αποτελούνται από γενικά πολυτοπικά στοιχεία. Τα στοιχεία γενικού σχήματος προσφέρουν μεγάλη ευελιξία στους πρακτικούς υπολογισμούς και μειώνουν το υπολογιστικό κόστος που απαιτείται για την εκλέπτυνση και την πύκνωση του πλέγματος. Η εκλέπτυνση των απότομων χρονικά εξαρτώμενων διεπιφανειών παραμένει μια σημαντική πρόκληση για το κομμάτι των υπολογισμών. Η ελευθερία στη γεωμετρία του πλέγματος σε συνδυασμό με τοπικά πολυώνυμα μεταβλητής τάξης ανά στοιχείο, αναμένεται να επιφέρει ακριβή προσέγγιση και ταυτόχρονα σημαντική μείωση του μεγέθους των συστημάτων προς επίλυση σε κάθε χρονικό βήμα.

Η νέα εκ των υστέρων ανάλυση σφαλμάτος του προβλήματος Allen-Cahn που παρουσιάζεται στα Κεφάλαια 3 και 4 φαίνεται να είναι αξιοποιήσιμη στο πλαίσιο του βέλτιστου ελέγχου. Πράγματι, μπορούμε να ξεκινήσουμε με το χαμηλής τάξης πλήρως διακριτό σύστημα, την ανάδρομη μέθοδο Euler - πεπερασμένων στοιχείων (dG(0) λόγω της χαμηλής ομαλότητας στα πλαίσια του βέλτιστου ελέγχου). Τουλάχιστον κατόπιν μικρών τροποποιήσεων, μπορούμε να εφαρμόσουμε τις εκ των υστέρων εκτιμήσεις στην εξίσωση κατάστασης. Ωστόσο, η κύρια πρόκληση είναι η απόδειξη (υπό συνθήκη ή όχι) εκ των υστέρων εκτιμήσεων σφαλμάτος της αντίστοιχης διακριτής εξίσωσης συζυγούς κατάστασης (5.16). Εξακολουθεί να διερευνάται η κατάλληλη τεχνική προσέγγισης του σφαλμάτος σε αυτή την περίπτωση. Θα εφαρμόσουμε τεχνικές σφαλμάτος για παραβολικές ΜΔΕ συγκρίνοντας άμεσα τη διαφορά μεταξύ της προσέγγισης (6.44) και της ακριβούς λύσης (5.16) ή είναι προτιμότερο να αναλύσουμε το ολικό σφάλμα μέσω μιας κατάλληλα ορισμένης χωροχρονικής ανακατασκευής;

Η εξίσωση συζυγούς κατάστασης είναι μια γραμμικοποιημένη παραβολική ΜΔΕ γύρω από τη λύση της εξίσωσης κατάστασης. Σε μια πρώτη σκέψη μπορούμε

να υποθέσουμε ότι δεν υπάρχει ανάγκη για ένα μη γραμμικό λήμμα Gronwall (μη κλασικό επιχείρημα συνέχειας). Ωστόσο, υπάρχουν δύο βασικά ζητήματα που πρέπει να ληφθούν υπόψη. Θα μελετήσουμε το σφάλμα στην $L_4(0, T; L_4(\Omega))$ -νόρμα; Αν μας ενδιαφέρει αυτή η κατεύθυνση, θα πρέπει να ορίσουμε μια συνάρτηση δοκιμής που θα αναδείξει την $L_4(0, T; L_4(\Omega))$ -νόρμα, αφού σε αντίθεση με την εξίσωση κατάστασης (εξίσωση Allen-Cahn) δεν είναι μια φυσικά προκύπτουσα νόρμα. Πώς μπορούμε να εξάγουμε εκ των υστερων εκτιμήσεις σφάλματος που εξαρτώνται πολυωνυμικά από το αντίστροφο του μήκους $1/\epsilon$ της διεπιφάνειας χωρίς να οδηγηθούμε σε επιπλέον συνθήκη με μεγαλύτερη εξάρτηση από το ϵ σε σχέση με την αντίστοιχη συνθήκη στην ανάλυση σφάλματος του προβλήματος κατάστασης;

Εφόσον αποδειχθούν εκ των υστερων εκτιμήσεις του προβλήματος συζυγούς κατάστασης, μπορούν να συνδυαστούν στη συνέχεια με τις αντίστοιχες εκτιμήσεις του προβλήματος κατάστασης προκειμένου να προκύψουν οι εκ των υστερων εκτιμήσεις του σφάλματος ελέγχου, $\bar{u} - \bar{u}_\sigma$. Πάλι, οι ικανές συνθήκες δεύτερης τάξης θα είναι το συνδετικό επιχείρημα. Ωστόσο, είναι απαραίτητο να επαναθεωρηθεί ώστε να είναι εφαρμόσιμες με εκ των υστερων τρόπο ως προς τον διακριτό βέλτιστο έλεγχο \bar{u}_σ .

Αν κάποιος ενδιαφέρεται να υπολογίσει το σφάλμα ελέγχου σε διαφορετικές νόρμες από την $L_2(0, T; L_2(\Omega))$, θα πρέπει να επιστρέψει και να αναδιατυπώσει το συγκεκριμένο πρόβλημα βέλτιστου ελέγχου. Η πρώτη εύλογη σκέψη είναι να επανεξετάσουμε το ενεργειακό συναρτησιακό ή/και το επιτρεπτό σύνολο U_{ad} . Ακόμη, ένα πιθανό σενάριο, σύμφωνα με το προφίλ της λύσης Allen-Cahn στις εξελισσόμενες διεπιφάνειες, είναι ο λεγόμενος έλεγχος *bang-bang* (για $\mu = 0$), όπου οι τιμές $\bar{u}(t, x)$ συμπίπτουν σχεδόν πάντοτο με μία από τις τιμές u_a ή u_b .

Η μελέτη άλλων προβλημάτων πεδίου φάσης είναι το επόμενο βήμα. Πιο συγκεκριμένα, είναι από μόνο του ενδιαφέρον να μελετηθεί κατά πόσο τα ήδη προτεινόμενα αριθμητικά σχήματα και οι τεχνικές που χρησιμοποιήθηκαν μπορούν να εφαρμοστούν (ίσως με κάποιες τροποποιήσεις) στις εξισώσεις Ginzburg-Landau, Cahn-Hilliard, Cahn-Larché. Η θεωρία που παρουσιάζεται στην παρούσα εργασία και εστιάζεται ιδιαίτερα στην μελέτη της $L_4(0, T; L_4(\Omega))$ -νόρμας αποτελεί ένα πιθανό σημείο εκκίνησης για τη διερεύνηση των προαναφερθέντων μοντέλων πεδίου φάσης λόγω της παρουσίας του διπλού δυναμικού.