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Modelling and Simulation for Brittle Fracture of Thin Shells subject to Normal Displacements

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Vollständiger Abdruck der von der Fakultät für Mathematik der Technischen Universität München zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften (Dr. rer. nat.)

genehmigten Dissertation

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   (nur schriftliche Beurteilung)

Die Dissertation wurde am 16.05.2019 bei der Technischen Universität München eingereicht und durch die Fakultät für Mathematik am 07.10.2019 angenommen.

Acknowledgement

First of all I say thank you to my supervisor Massimo Fornasier, who made my dissertation at all possible by accepting my application at TUM and by offering me a doctoral position within the IGDK. He always believed in my abilities to become a researcher and to successfully finish my doctoral studies. His chair, M15, provided a great working environment with an interdisciplinary and international research group. It was a pleasure to work among all these nice colleagues. Especially, Stefano Almi was not only a great research companion but also became a true friend. It is hard to see how I could have finished my research projects without him. Another thank goes to the chair's secretary, Silvia Toth-Pinter, who was always very friendly and helpful.

My position during the last three and a half years was financed by the DFG through the International Research Training Group IGDK 1754 "Optimization and Numerical Analysis for Partial Differential Equations with Nonsmooth Structures". I acknowledge the effort of Boris Vexler, the speaker of the IGDK at TUM, and of its administrative coordinator, Diane Clayton-Winter, who was extremely helpful and supportive at any time. The IGDK made it possible for me to visit many summer schools, conferences and seminars as well as to arrange several international collaborations. Within its program I spend 6 month at University of Graz. Collaborating with Kristian Bredies I had a very efficient and motivating time, which I appreciate a lot.

During my studies at TUM I regularly visited Stefano Micheletti and Simona Perotto at Polytechnic University of Milan. I thank both for their hospitality, their support and their time. I am very happy about the achieved results. Furthermore, I give thanks to Matteo Negri from University of Pavia and his collaboration. I send a big thanks to the referees of this thesis and the whole examining committee for their work.

Last but not least I thank my family, particularly my parents and my three brothers. They never doubted of me, and they always supported every aim I had in my life.

Abstract

In this work we derive a two-dimensional variational brittle fracture model of Mumford-Shah type for parametrized surfaces. Starting with the three-dimensional Francfort-Marigo model for brittle fracture of a given surface endowed with a thickness, we transform the energy functional to curvilinear coordinates, restrict – for simplicity – the addmissible displacements to those which are orthogonal to the given surface, and compute the Γ-limit as the thickness tends to zero.

We then provide a broad generalization of the well-known Ambrosio-Tortorelli approximation for the Mumford-Shah functioal. With this at hand we obtain a phase field model for our new fracture model of thin shells. Apart from the main theme of this thesis we additionally show a second phase field approximation which allows the phase field to be a function of bounded variation. We do not apply this to fracture mechanics but present some numerical results in the context of segmental image denoising.

Further, for the new fracture phase-field model we study time evolutions driven by a time-dependent boundary condition. Precisely, we introduce a new time-discrete alternating minimization scheme, where we implement the irreversibility of the crack via a pointwise minimization of the phase-field variable. Subsequently we prove the convergence of this scheme to a unilateral L^2-gradient flow as the time step size converges to zero. Additionally we show its consistency with finite element discretizations.

In the last part of this thesis we put together all the previous pieces and compute some numerical simulations of fracture propagations on thin shells. Based on some residual estimate we use for this simulations an anisotropic mesh adaption procedure.

Zusammenfassung

In dieser Arbeit leiten wir ein zwei-dimensionales variationelles Modell für spröde Brüche für parametrisierte Oberflächen im Sinne des Mumford-Shah Modells her. Wir starten mit dem drei-dimensionalen Francfort-Marigo Modell für spröde Brüche einer gegebenen Oberfläche ausgestattet mit einer Dicke. Wir transformieren das Energie-Funktional in kurvenförmige coordinaten, schränken – der Einfachheit halber – die zulässigen Verformungen auf solche ein, die orthogonal zur gegebenen Oberfläche sind und berechnen das Γ-Limit, wenn die Dicke gegen null konvergiert.

Wir stellen anschließend eine umfassende Verallgemeinerung der bekannten Ambrosio-Tortorelli Approximation des Mumford-Shah Funktionals zur Verfügung. Damit erhalten wir ein Phasenfeld-Modell für unser neues Bruch-Modell dünner Hüllen. Abseits des Hauptthemas dieser Dissertation zeigen wir außerdem eine weitere Phasenfeld-Approximation, die es der Phasenfeld erlaubt eine Funktion von beschränkter Variation zu sein. Wir wenden dies nicht auf die Bruchmechanik an sondern präsentieren einige numerische Resultate im Kontext segmentaler Bildentrauschung.

Des Weiteren untersuchen wir für das neue Phasenfeld-Modell für Brüche Zeitentwicklungen, angetrieben durch eine zeitabhängige Dirichlet Randbedingung. Genau genommen führen wir ein neues zeitdiskretes Verfahren alternierender Minimierung ein, indem wir die Irreversibilität des Bruches durch eine punktweise Minimierung der Phasenfeld-Variablen realisieren. Daraufhin beweisen wir die Konvergenz des Verfahrens gegen ein unilateralen L^2-Gradienten-Fluss, wenn der Zeitschritt gegen null konvergiert. Außerdem zeigen wir dessen Konsistenz mit einer Finite-Elemente-Diskretisierung.

Im letzten Teil dieser Dissertation fügen wir alle vorherigen Stücke zusammen und berechnen einige numerische Simulationen von Bruchentwicklungen auf dünnen Hüllen. Basierend auf Rest-Abschätzungen nutzen wir für diese Simulationen ein Verfahren zur anisotropen Gitteradaption.

Contents

1 Introduction

The history of modern fracture mechanics goes back to the 1920s. A. A. Griffith worked during the First World War in this field and established some fundamental laws in [77], which can be seen as the beginning of the contemporary theory of fracture mechanics. In short, he considered elastic materials and ascertained that the surface energy which refers to the energy stored along the crack, is proportional to the crack length. The constant of proportionality is called the *toughness*. Griffith's theory is mainly applicable to brittle materials, that means to materials which are not permanently deformed before breaking. In other terms the material is fully elastic. Examples are glass or ceramic. The first one was the material Griffith was actually working with. In contrast to brittle materials there are the so called ductile ones, which are permanently deformed before they actually break. Focusing on materials such as steel, where Griffith's theory failed, G. R. Irwin further developed Griffith's theory by introducing a plastic zone around the crack tip (see [81]). Since in this thesis, we focus on ideally purely brittle materials we are not going into further details here. Instead, we jump to the end of the 20th century, when the mathematical model, as we will use it here, was introduced.

In 1998 G. A. Francfort together with J.-J. Marigo introduced in [68] a variational model, for modelling brittle fracture in the sense of Griffith, which is frequently used until nowadays. Given a specimen, they considered the total energy as the sum of the elastic energy, depending on the displacement of this specimen, and the surface energy, depending on the set describing the crack. Minimizing this energy functional, under some forced boundary conditions, then yields a stable equilibrium state of the system. However, there is some drawbacks lying in the physical laws formulated by Griffith. That is, crack initialization is theoretically not possible (see e.g. [31, 68]). We will find this issue again in this thesis, since we always assume the existence of an initial crack.

Before getting into more details, for which we need to become also mathematically more technical, we mention some rather surprising fact. That is that the energy functional of Francfort and Marigo already appeared in 1989 in a very different context. D. Mumford and J. Shah had been used the more or less same model in [97] for segmental image denoising, which is the reason that the energy functional is often called *Mumford-Shah functional*. Instead of the displacement, here the function is the grey level of a picture, whereas the fracture set represents the edges separating the different segments in the image. Because these two fields are closely related – at least from a mathematical point of view – some result in this thesis is also applied to segmental image denoising. Nevertheless, the main focus of this thesis remains on fracture mechanics.

1.1 The Mumford-Shah Functional

We start with the mathematical details about the Mumford-Shah functional in the context of segmental image denoising, as this is the historical order and somehow simpler than in the application of fracture mechanics. As already mentioned, the Mumford-Shah functional has been introduced in [97] in the context of segmental image denoising. Imagine a gray image, modeled by the function $g \in L^\infty(\Omega)$, where $\Omega \subset \mathbb{R}^n$ represents the image domain, and one wants to denoise the image without becoming blurred along high contrast lines. In mathematical terms this means that our model should detect these edges of high contrast, along which the approximated image is allowed to jump. In the cited paper the authors suggested to minimize the following functional with respect to the function u, describing the denoised image, and the set Γ, describing the edges:

$$\frac{\alpha}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{\beta}{2}\int_\Omega |u-g|^2, \,\mathrm{d}x + \gamma \mathcal{H}^{n-1}(\Gamma) \tag{1.1}$$

where $\alpha, \beta, \gamma > 0$ are parameters, free to choose. To be more precise $\Gamma \subset \mathbb{R}^n$ is an $n-1$-dimensional closed set and $u \in C^1(\Omega \setminus \Gamma)$. Let us briefly describe the different terms of this functional, which can be weighted differently by the parameters α, β and γ. The first integral of this functional is responsible for the denoising effect. The larger α is the smoother becomes u, i.e. the less noise remains. The second integral ensures that u is similar to the original picture g and the last part weighted by γ measures the length of the detected edges, i.e. γ controls how sensitive the model is concerning the contour detection. Clearly, these paramters need to be chosen with care in order to get a sensible result. Some numerically computed examples of minimizers of the Mumford-Shah functional can be found in Section 4.4.

For modelling brittle fractures the functional in (1.1) needs to be modified. The domain $\Omega \subset \mathbb{R}^n$ now describes the specimen. The two-dimensional closed set $\Gamma \subset \mathbb{R}^n$ describes the crack. In general now u is a vector valued function, which describes the displacement of the specimen. Moreover, the first integral is replaced by the elastic energy and the second integral is removed completely, i.e. $\beta = 0$. Instead one imposes some Dirichlet boundary condition, say $g \in C^1(\partial\Omega; \mathbb{R}^n)$, on u. Altogether one wants to minimize the functional

$$\frac{1}{2}\int_\Omega \boldsymbol{C}\boldsymbol{\epsilon} u : \boldsymbol{\epsilon} u \,\mathrm{d}x + \kappa \mathcal{H}^{n-1}(\Gamma) \tag{1.2}$$

with respect to Γ and $u \in C^1(\Omega; \mathbb{R}^n)$ such that $u = g$ on $\partial\Omega$. Here, we used linear elasticity, where $\boldsymbol{C}$ is the stiffness tensor and $\boldsymbol{\epsilon} u = \frac{1}{2}(\nabla u^\top + \nabla u)$ is the symmetric gradient. The operator : stands for the tensor product. Throughout, this thesis we only consider linear elasticity, which is a good approximation for small deformations. Without going into details, for the mathematical modelling of elasticity we refer to the extensive monograph [47]. The second term of this energy functional now measures the surface created by the crack Γ where κ is the toughness of the material which is always considered to be constant for the rest of this work.

Starting from this model, we will derive in Chapter 3 a two-dimensional fracture model for curved surfaces. This is achieved by using the full three-dimensional functional (1.2) for a given surface endowed with a thickness. Then we investigate the limit as the thickness goes to zero. Actually, we make a further simplification by restricting the admissible vector fields describing the displacement to those, which are orthogonal to the given surface. In this way things become a bit simpler, since we can deal with a real valued function, measuring the length of the orthogonal deformation at each point. With further details we wait for Chapter 3.

Thinking of plates as the given surfaces, that are only deformed in their orthogonal direction, we end up with the well-known anti-plane strain setting. This means that $\Omega \subset \mathbb{R}^2$ is a flat plate embedded in $\mathbb{R}^3$ and the displacement is restricted to be orthogonal to the plate, so that u is real valued again. The elastic energy then reduces to a simpler term, such that the total energy in (1.2) becomes

$$\frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \kappa \mathcal{H}^{n-1}(\Gamma)\,. \tag{1.3}$$

This is again the Mumford-Shah functional from (1.1) with $\beta = 0$.

The difficulty in minimizing these problems is the dependency of the set Γ, where u is allowed to be discontinuous. Due to this fact such problems are also called *free-discontinuity problems.*

In order to show the existence of minimizers of this functional, a natural idea is to use the direct method of variational calculus. This, however, requires to have a suitable topology in which some minimizing sequence attains at least one limit point. A first try would probably be to suggest the topology for sets, which is induced by the Hausdorff metric. Unfortunately, this approach is doomed since the functional is not lower semi-continuous with respect to this topology. Particularly, for a sequence (Γ_k) converging to Γ with respect to the Hausdorff metric, there does generally *not* hold (see [10, Section 6.1])

$$\mathcal{H}^{n-1}(\Gamma) \le \liminf_{k\to\infty} \mathcal{H}^{n-1}(\Gamma_k)\,.$$

The help is coming from an idea, which is by now standard in the theory of free-discontinuity problems (see [10, 34]). One relaxes the function space $C^1(\Omega \setminus \Gamma)$ to the space of *special functions of bounded variations*, written as $\mathrm{SBV}(\Omega)$. We recall the definition and some properties of this space in Section 2.4. For now, the reader can imagine that this function space contains piecewise (H^1-)smooth functions, where the set of discontinuity, denoted by S_u, is a two-dimensional (but not necessarily closed) set, which replaces Γ. Namely, instead of (1.1) one considers

$$\frac{\alpha}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{\beta}{2}\int_\Omega |u-g|^2 \,\mathrm{d}x + \gamma \mathcal{H}^1(S_u) \tag{1.4}$$

for $u \in \mathrm{SBV}(\Omega)$. In [6, 7, 8] it has been proven that the space $\mathrm{SBV}(\Omega)$ fulfills some nice compactness properties ensuring that the minimizing sequence has a limit point in $\mathrm{SBV}(\Omega)$ (with respect to the weak*-convergence in $\mathrm{BV}(\Omega)$) and the functional is lower semi-continuous along this sequence. Hence, the direct method can be applied, and the existence of minimizers of (1.4) follows. Furthermore, by the regularity property shown in [58] we know that for any minimizer $u \in \mathrm{SBV}(\Omega)$ of (1.4) the pair $(u, \bar{S}_u)$ minimizes (1.1).

Note, that when $\beta = 0$ – which is the case in anti-plane fracture mechanics (1.3) – the functional must be defined on $\mathrm{GSBV}(\Omega)$, the set of *generalized special functions of bounded variation* (see Section 2.4 for more details on these functions), in order to obtain the existence of a minimizer. This is due to the requirement of a uniform bound of the minimizing sequence in the direct method for applying the mentioned compactness properties in $\mathrm{SBV}(\Omega)$. Only for $\beta > 0$ this bound is automatically achieved, whereas for $\beta = 0$ one has to fall back to $\mathrm{GSBV}(\Omega)$. The weak formulation of (1.3), therefore, writes like

$$\mathcal{MS}(u) := \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \kappa \mathcal{H}^{n-1}(S_u)\,, \tag{1.5}$$

for $u \in \mathrm{GSBV}(\Omega)$.

Moreover, when u is vector valued, which is the case in (1.2), the right spaces for achieving the existence of minimizers are even more complicated, and one has to define the functionals on *(generalized) special functions of bounded deformation*, usually denoted by $\mathrm{SBD}(\Omega)$ respectively $\mathrm{GSBD}(\Omega)$. In this work we do not really make use of this spaces and we are satisfied with referring to [9, 54, 103] for more details.

1.2 Time Evolutions

One crucial difference between the image and fracture model, which we have not discussed so far, is that in imaging one clearly has a static problem, whereas in fracture mechanics we are interested in time evolutions. Particularly, one wishes to observe the crack propagation depending on some time dependent load, here a time dependent Dirichlet boundary condition for the admissible displacement. At this point, we focus on *quasi-static* evolutions, that is we assume that the system is at each time in an equilibrium state. As we have to stay rather brief with the details of this theory, the reader shall be referred to [31], a very comprehensive work on quasi-static time evolutions of different variational models.

In general the term “equilibrium state” can refer to global or local minimizers or even only to critical point of the considered energy functional, where the latter seems to be the most physical approach, at least when the crack path is defined a priori (see [31, Proposition 2.1]). When the crack path is free to propagate in any direction, the terms “local minimum” or “critical point” of (1.2) require some specified topology in order to give sense to these terms. As we have seen above, when considering the strong formulation (1.3) such a topology is not easy to find. However, a global minimizer is independent of any topology and the existence is guaranteed from the discussion above. From a mathematical perspective it is, therefore, easier to consider global minimizers, which was also the first approach of [68] when defining quasi-static time evolution.

Beside the required equilibrium, physics and mathematics demands more conditions from an admissible time evolution. Already in Griffith's theory one can find the *irreversibility condition*, stating that once a crack is present it can not disappear and repair itself. In mathematical terms, considering the crack set Γ as a function of time, we express this condition by $\Gamma(t) \subset \Gamma(s)$ for all $s < t$. Furthermore, one requires some regularity condition on the total energy as well as the description of its evolution in time. We then obtain a quasi-static evolution as it has been introduced in [68]: Suppose a Dirichlet boundary condition g on a part of the boundary of the domain Ω, say $\partial_D\Omega$, that varies in time $t \in [0,T]$ (for some final time $T > 0$). Then, the quasi-static evolution $t \mapsto (u(t), \Gamma(t))$ is defined by the following conditions:

[TE1] Γ is increasing in time, i.e. $\Gamma(t) \subset \Gamma(s)$ for all $0 \le s \le t \le T$.

[TE2] For every $t \in [0,T]$ the couple $(u(t), \Gamma(t))$ is a global minimizer of the energy functional (1.3) among all u and Γ, such that $u = g$ on $\partial_D\Omega$ and $\bigcup_{s<t} \Gamma(s) \subset \Gamma$.

[TE3] The energy $t \mapsto \frac{1}{2}\int_\Omega |\nabla u(t)|^2 \,\mathrm{d}x + \kappa\mathcal{H}^{n-1}(\Gamma(t))$ is absolutely continuous in time and its derivative is equal to the power of external forces.

The translation of this notion to the weaker formulation (1.5) is not that obvious. We cannot simply replace Γ by S_u. If the boundary conditions are changing it is imaginable that u might become continuous at some point where it was discontinuous before, which would lead to a contradiction to the irreversibility condition. The solution is to identify the crack at a specific time by the union of all previous discontinuity sets of u. The idea comes from [69], where the authors define a quasi-static evolution $t \mapsto u(t) \in \mathrm{GSBV}(\Omega)$ with respect to (1.5). Setting

$$\Gamma(t) := \bigcup_{s<t} \Big(S_{u(s)} \cup \big(\partial_D\Omega \cap \{u(s) \neq g(s)\}\big) \Big) \quad \text{for all } t \in [0,T]$$

they require the following properties:

[TE4] For every $t \in [0,T]$ and for all $z \in \mathrm{GSBV}(\Omega)$ there holds

$$\frac{1}{2}\int_\Omega |\nabla u(t)|^2 \,\mathrm{d}x + \kappa\mathcal{H}^{n-1}(\Gamma(t)) \le \frac{1}{2}\int_\Omega |\nabla z|^2 \,\mathrm{d}x + \kappa\mathcal{H}^{n-1}\Big(S_z \cup \big(\partial_D\Omega \cap \{z \neq g(t)\}\big) \cup \Gamma(t)\Big).$$

[TE5] The energy $\mathcal{E}(t) := \frac{1}{2}\int_\Omega |\nabla u(t)|^2 \,\mathrm{d}x + \kappa\mathcal{H}^{n-1}(\Gamma(t))$ is absolutely continuous in time and there holds

$$\mathcal{E}(t) = \mathcal{E}(0) + \int_0^t \int_\Omega \nabla u(s) \nabla \dot{g}(s) \,\mathrm{d}x \,\mathrm{d}s\,.$$

Note that the irreversibility condition is implicitly fulfilled by the definition of $\Gamma(t)$. In [69] the existence of such evolutions is showed.

1.3 Phase Field Models

Knowing the existence of quasi-static time evolutions or global minimizers of the functional $\mathcal{MS}$ from (1.5) still does not answer, how actually to compute them. A crucial break through for numerical computations has been given by L. Ambrosio and V. M. Tortorelli in [12, 13]. Inspired by the work [96] they introduced some elliptic phase field approximation in terms of Γ-*convergence*.

Precisely, they introduced for $\varepsilon > 0$ the functionals

$$\mathcal{AT}_\varepsilon(u,v) := \frac{\alpha}{2}\int_\Omega (v^2+\eta_\varepsilon)|\nabla u|^2 \,\mathrm{d}x + \int_\Omega \frac{1}{4\varepsilon}(1-v)^2 + \varepsilon|\nabla v|^2 \,\mathrm{d}x \tag{1.6}$$

for $u \in H^1(\Omega)$ and $v \in H^1(\Omega;[0,1])$ and showed via a Γ-convergence argument that any limit point $(u,1)$ of a sequence of minimizers $(u_\varepsilon, v_\varepsilon)$ of $\mathcal{AT}_\varepsilon$ is a minimizer of (1.5), provided that $\frac{\eta_\varepsilon}{\varepsilon} \to 0$. We recall some details about Γ-convergence in Section 2.3. The additionally introduced dummy variable v works as a *phase field* variable describing the discontinuity set of u. In particular, in (1.6), the function v takes values in the interval $[0,1]$, where $v(x) = 1$ means that the elastic body is safe at $x \in \Omega$, while $v(x) = 0$ means that the material is fractured at x.

In the last years, after [27], the use of phase field models in computational fracture mechanics has been constantly increasing (see, e.g., [5] for a review on different models). From the computational stand point, the study of the functional (1.6) is very convenient in combination with the so-called alternate minimization, also known as Gauss-Seidel iteration scheme. In [27], and many subsequent works like [16, 38], equilibrium configurations of the energy are indeed computed iteratively, minimizing $\mathcal{AT}_\varepsilon$ first with respect to u and then with respect to v. In this way, at each iteration we look for a minimum of a quadratic functional, which leads, in the numerical framework, to solve a linear system. Moreover, energies like $\mathcal{AT}_\varepsilon$, defined in Sobolev spaces, can be easily discretized in finite element spaces or, alternatively, by finite differences.

However, the phase field approach raises several questions, of interest both on the theoretical level and for the applications. First, it is important to understand the relationship between phase field and sharp crack energies, obtained in the limit as $\varepsilon \to 0$. The Γ-convergence guarantees that global minimizers of (1.6) converge to global minimizers of (1.5), under suitable compactness properties.

Second, we would like to know the connection between suitable time evolutions of phase-field models and those described in the previous section for the sharp model. The first known result goes back to [75]. A. Giacomini implemented the irreversibility condition in the phase-field model by forcing the phase field to be decreasing in time. Precisely, he says that $t \mapsto (u_\varepsilon(t), v_\varepsilon(t)) \in H^1(\Omega) \times H^1(\Omega;[0,1])$ is a quasi-static time evolution of the phase field model $\mathcal{AT}_\varepsilon$ for $\varepsilon > 0$ driven by a time dependent boundary condition $g(t)$ on $\partial_D\Omega$ if there holds

[TE6] $v_\varepsilon(t) \le v_\varepsilon(s)$ for all $s < t$.

[TE7] $\mathcal{AT}_\varepsilon(u_\varepsilon(t), v_\varepsilon(t)) \leq \mathcal{AT}_\varepsilon(u,v)$ for all $u \in H^1(\Omega)$, $v \in H^1(\Omega;[0,1])$ with $u = g(t)$, $v = 1$ on $\partial_D\Omega$ and $v \leq v_\varepsilon(t)$.

[TE8] for $\mathcal{E}_\varepsilon(t) := \mathcal{AT}_\varepsilon(u_\varepsilon(t), v_\varepsilon(t))$ is absolutely continuous in time and

$$\mathcal{E}_\varepsilon(t) = \mathcal{E}_\varepsilon(0) + \int_0^t \int_\Omega (\eta_\varepsilon + v_\varepsilon^2(s))\nabla u_\varepsilon(s)\nabla \dot{g}(s)\,\mathrm{d}x\,\mathrm{d}s$$

[TE9] for some constant $C > 0$ there holds $\mathcal{E}_\varepsilon(t) \leq C$ for all $t \in [0,T]$.

Property [TE6] corresponds to the irreversibility condition. Property [TE7] represents the equilibrium condition in terms of global minimizers at each time. Property [TE8] describes the time evolution of the phase field energy; and property [TE9] is more a technical condition in order to obtain some compactness properties when $\varepsilon \to 0$.

Now A. Giacomini could prove that evolutions of the phase field model in the sense of [TE6]–[TE9] converge to time evolutions of the sharp model in the sense of [TE4]–[TE5] as ε tends to zero.

At the present stage not much is known about the convergence of critical points of $\mathcal{AT}_\varepsilon$ to critical points of $\mathcal{MS}$. This is related to the fact that a "good" notion of energy release or slope in BV-like spaces is still missing (see, e.g., [57]). For this reason it is also not clear where quasi-static evolutions along critical points of phase field models converge to. Some result in one dimension is available in [70].

Nevertheless, hoping for the best it has been common practice to study time evolutions (along critical points) of the phase field models by its own. This is also due to the fact that using the alternating minimization in numerical computation results in critical points of $\mathcal{AT}_\varepsilon$ and one can not expect to get global minimizers. Further, regarding some necessary time discretization of these such algorithms, one needs to investigate the convergence behaviour as the time step goes to zero (see e.g. [87]). When taking also a space discretization into account, things become even more complex. Together with S. Almi we could show the consistency of a finite element discretization in the alternating minimization in order to obtain quasi-static evolutions along critical points of the phase field model (see [2]). We do not present this work in this thesis, instead we focus on a similar research which was developed together with S. Almi and M. Negri in [1]: In Chapter 5 we present another form of time evolutions of phase field models, that is a unilateral L^2-gradient flow and show the convergence of a modified time-discretized alternating minimization as the time increment tends to zero. The theory also includes the consistency check of a space discretization by a finite element method.

1.4 Structure of the Thesis

We keep this introduction quite short and give deeper insides at the beginning of each chapter to the specific topics discussed therein. At this point let us only summarize the structure of this thesis. We start in Chapter 2 with some preliminaries concerning some theoretical basics, which are useful for this thesis, including some notational conventions.

In Chapter 3 we develop the two-dimensional fracture model by a Γ-convergence argument, passing from three to two dimension. As far as we know this is the first time that such a fracture model for general curved surfaces is presented. The theory in there has been deduced with the advice of S. Almi and is planed to be published in [4].

In the first part of Chapter 4 we present a broad generalization of the phase field model from Ambrosio and Tortorelli. As a specific case we obtain in this way also an approximation for our new two-dimensional energy of brittle thin shells. Also this part has been derived with the help of S. Almi. It is planed to be published in [3]. The second part of this chapter is the content of the submitted paper [23]. In collaboration with K. Bredies we have developed a model, where the phase field variable is allowed to be a function of bounded variation. We compare this result numerically with the traditional approximation from Ambrosio and Tortorelli in the context of segmental image denoising. There, one can observe that our new model results in sharper edge detections.

We discuss time evolutions of the generalized phase field approximation of the brittle thin shells in Chapter 5. It is based on the paper [1], which was written in collaboration with S. Almi and M. Negri. Therein, we show the convergence of some alternating minimization to a unilateral L^2-gradient flow. Besides the time discretization we also take care of the consistency with a finite element discretization of the space. Another investigative idea is the implementation of the irreversibility condition by a point wise minimization of the phase field variable. The content of the paper was adapted for this thesis in order to fit to the setting of our thin shell model.

The purpose of the last chapter, Chapter 6, is the presentation of some numerical simulation of brittle fracture propagation of thin shells, which have been set up with the help of S. Micheletti and S. Perotto. Up to our knowledge and investigation these are the first numerical experiments of fracture on curved surfaces. Additionally, we make use of an anisotropic mesh adaption procedure based on some residual estimates, which we also compute in this thesis. This part is planed to be published together with Chapter 3 in [4].

2 Preliminaries

In this section, we collect the notation and the well-known results which are used in this thesis. We start with some basic notational conventions in tabular form.

2.1 Basic Notation

We start with some basic sets and abbreviations:

$\mathbb{N}$	is the set of all natural numbers (without 0).
$\mathbb{N}_0$	is the set of all nonnegative integers, $\mathbb{N} \cup \{0\}$.
$\mathbb{R}$	denotes the set of all real numbers.
$\mathbb{1}$	is the constant one function.
a.a.	stands for the term "almost all".
a.e.	stands for the term "almost everywhere".

For $n \in \mathbb{N}$, $a, b \in \mathbb{R}$ and for a (possibly signed and vector valued) measure μ on $\mathbb{R}^n$ we write

$\mathbb{R}^n$	for the standard n-dimensional Euclidean space.
$\mathbb{S}^{n-1}$	for the $n-1$-dimensional unit sphere with respect to the Euclidean norm, embedded in the n-dimensional Euclidean space.
$a \vee b$, $\max\{a, b\}$	for the maximum of a and b.
$a \wedge b$, $\min\{a, b\}$	minimum of a and b.
$\mathcal{L}^n$	for the n-dimensional Lebesgue measure.
$\mathcal{H}^n$	for the n-dimensional Hausdorff measure.
$\#$	for the counting measure, i.e. for $\mathcal{H}^0$.
$\lvert\mu\rvert$	for the total variation of μ.

For some points $x, y \in \mathbb{R}^n$ and a subset $\Omega \subset \mathbb{R}^n$ we use the symbol

$\lvert x\rvert$	for the standard Euclidean norm of x.
$\langle x, y\rangle$, $x \cdot y$	for the standard scalar product of x and y.
$\operatorname{dist}(\Omega, x)$	for the Euclidean distance of x from Ω, $\operatorname{dist}(\Omega, x) =$.
$\overline{\Omega}$	for the closure of Ω.
$\partial\Omega$	for the topological boundary of Ω.

$\Omega^\perp$	for the orthogonal complement of Ω with respect to the standard scalar product.
$B_r(x)$	for the open ball with centre x and radius r with respect to the Euclidean distance.
$B_r(\Omega)$	for the open r-neighbourhood of Ω with respect to the Euclidean distance.
$\pi_\Omega(x)$	for the projection of x onto Ω.
χ_Ω	for the characteristic function of Ω.

Let $n, k, d \in \mathbb{N}$ and $\Omega \subset \mathbb{R}^n$, $W \subset \mathbb{R}^d$ and $1 \leq p \leq \infty$. Then we use the following standard function spaces:

$L^p(\Omega; W)$	is the space containing all functions $f\colon \Omega \to W$ such that $\lvert f\rvert^p$ is integrable on Ω.
$W^{p,k}(\Omega; W)$	is the Sobolev space, consisting of all functions in $L^p(\Omega; W)$ whose weak derivatives up to order k are all in $L^p(\Omega)$
$W_0^{p,k}(\Omega; W)$	is the Sobolev space, consisting of all functions in $W^{p,k}(\Omega; W)$ with value zero at the boundary (in the sense of traces).
$H^k(\Omega; W)$	denotes the Sobolev space $W^{2,k}(\Omega)$.
$H_0^k(\Omega; W)$	denotes the Sobolev space $W_0^{2,k}(\Omega)$
$L^p(\Omega)$	is an abbreviation for $L^p(\Omega; \mathbb{R})$.
$W^{p,k}(\Omega)$	is an abbreviation for $W^{p,k}(\Omega; \mathbb{R})$.
$W_0^{p,k}(\Omega)$	is an abbreviation for $W_0^{p,k}(\Omega; \mathbb{R})$.
$H^k(\Omega)$	is an abbreviation for $H^k(\Omega; \mathbb{R})$.
$H_0^k(\Omega)$	is an abbreviation for $H_0^k(\Omega; \mathbb{R})$.
$\mathrm{BV}(\Omega)$	stands for the space of all real valued functions of bounded variation on Ω.
$\mathrm{SBV}(\Omega)$	stands for the space of all real valued special functions of bounded variation on Ω.
$\mathrm{GBV}(\Omega)$	stands for the space of all real valued generalized functions of bounded variation on Ω.
$\mathrm{GSBV}(\Omega)$	stands for the set of all real valued generalized special functions of bounded variation on Ω.
$\mathrm{BD}(\Omega)$	stands for the space of real valued functions of bounded deformation on Ω.
$\mathrm{SBD}(\Omega)$	stands for the space of real valued special functions of bounded deformation on Ω.
$\mathrm{GSBD}(\Omega)$	stands for the set of real valued generalized special functions of bounded deformation on Ω.
$\mathrm{SBV}^2(\Omega)$	stands for the space of all functions in $\mathrm{SBV}(\Omega)$ with finite $\mathcal{H}^{n-1}$ measure of S_u and square integrable approximate gradient.

$\mathrm{GSBV}^2(\Omega)$	stands for the space of all functions in $\mathrm{GSBV}(\Omega)$ with finite $\mathcal{H}^{n-1}$ measure of S_u and square integrable approximate gradient.

For a function $f\colon \mathbb{R}^n \to \mathbb{R}$ we write

f^*	for the convex conjugate of f.
f^{**}	for the biconjugate of f, which is its lower semi-continuous convex hull.
∇f	for the approximate gradient of the function f.
$\nabla^2 f$	for the Hessian of the function f.
$\mathrm{Var}(f, \Omega)$	for the variation of f on Ω.

As an overview we summarize here also the notation for functions of bounded variation, which is introduced in more detail in Section 2.4. For $u \in \mathrm{BV}(\Omega)$ we set the following:

$\mathrm{D}u$	denotes the distributional derivative of u, being a Radon measure.
$\mathrm{D}^{\mathrm{a}}u$	denotes the absolutely continuous part of $\mathrm{D}u$ with respect to the Lebesgue measure.
$\mathrm{D}^{\mathrm{j}}u$	denotes the jump part of the distributional derivative of u.
$\mathrm{D}^{\mathrm{c}}u$	denotes the cantor part of the distributional derivative of u.
S_u	denotes the discontinuity set of u.
u^+, u^-	denotes the upper, respectively lower, approximate limit of u.
ν_u	denotes the unit normal of a jump point, pointing in the direction of u^+.
$\tilde{u}$	denotes the precise representative of u

Before we go into more details in some topics we recall a well-known result about the gradient of a distance function. It follows from the proof of [62, 3.2.34].

Lemma 2.1.1. *Let $\Omega \subset \mathbb{R}^n$ be a closed set and denote the Euclidean distance to Ω by $\tau\colon \mathbb{R}^n \to \mathbb{R}$, i.e. $\tau(x) = \mathrm{dist}(\Omega, x)$. Then τ is differentiable almost everywhere with*

$$|\nabla\tau| = 1 \quad \textit{and, hence} \quad \nabla\tau(x) = \frac{x - \pi_\Omega(x)}{|x - \pi_\Omega(x)|}$$

where $\pi_\Omega(x)$ denotes the projection of x onto Ω, i.e. $\pi_\Omega(x) = \arg\min_{y\in\Omega}|x-y|$.

2.2 Convex Functions

Especially, for the numerical part of this paper we also need some theory about convex functions. A good reference for this topic is [80] and [60]. In this context it is sufficient to consider functions defined on the real line. All the discussed issues can easily be adapted to a multi dimensional setting.

Let therefore $I \subset \mathbb{R}$. The characteristic function over I is given by $\chi_I = 0$ on I and $\chi_I = +\infty$ on $\mathbb{R} \setminus I$. For any function $f\colon I \to \mathbb{R}$, bounded from below by some affine function, $f^*\colon \mathbb{R} \to \mathbb{R}$ denotes its convex conjugate, i.e.

$$f^*(s) = \sup_{t\in\mathbb{R}}\big(ts - f(t)\big) \quad \text{for all } s \in \mathbb{R}$$

where f is set to $+\infty$ outside of I. This definition directly yields Fenchel's inequality, which says

$$ts \le f(t) + f^*(s) \quad \text{for all } t, s \in \mathbb{R}\,. \tag{2.1}$$

We remark that f^* is always convex and lower semi-continuous and the biconjugate $f^{**} = (f^*)^*$ is the lower semi-continuous convex hull of f. Furthermore, f is convex and lower semi-continuous if and only if $f = f^{**}$.

2.3 Γ-convergence

For some sequence of functionals (F_j) and a functional F defined on some metric space X we say that F_j Γ-*converges* to F as $j \to \infty$ and write $\Gamma\text{-}\lim_{j\to\infty} F_j = F$ if there holds the following two conditions:

lim inf-inequality, i.e. for all $u \in X$ and all sequences (u_j) in X with $u_j \to u$ there holds

$$F(u) \le \liminf_{j\to\infty} F_j(u_j)\,.$$

lim sup-inequality, i.e. for all $u \in X$ there exists a sequence (u_j) in X such that $u_j \to u$ and

$$\limsup_{j\to\infty} F_j(u_j) \le F(u)\,.$$

One often defines

$$\Gamma\text{-}\liminf_{j\to\infty} F_j(u) := \inf\{\liminf_{j\to\infty} F_j(u_j)\colon u_j \in X \text{ for all } j > 0, u_j \to u \text{ as } j \to \infty\}\,,$$
$$\Gamma\text{-}\limsup_{j\to\infty} F_j(u) := \inf\{\limsup_{j\to\infty} F_j(u_j)\colon u_j \in X \text{ for all } j > 0, u_j \to u \text{ as } j \to \infty\}\,.$$

Then the lim inf-inequality is equivalent to $F \le \Gamma\text{-}\liminf_{j\to\infty} F_j$ and the lim sup-inequality is equivalent to $\Gamma\text{-}\limsup_{j\to 0} F_j \le F$. Note that $\Gamma\text{-}\liminf_{j\to\infty} F_j$ as well as $\Gamma\text{-}\limsup_{j\to\infty} F_j$ are lower semi-continuous.

If one has a family of functionals (F_ε) for $\varepsilon \in I \subset \mathbb{R}$ the definition is adapted in the usual way, i.e. F_ε Γ-converges to F as $\varepsilon \to a$ (for some $a \in \bar{I}$) if F_{ε_j} Γ-converges to F for all sequences (ε_j) in I with $\varepsilon_j \to a$.

The most important property of Γ-convergent sequences is the convergence of minimizers to a minimizer of the limit functional, which is stated in the following proposition.

Proposition 2.3.1. *Let $F_\varepsilon \colon X \to \mathbb{R} \cup \{\infty\}$ be a sequence of functionals Γ-converging to $F \colon X \to \mathbb{R} \cup \{\infty\}$, where X is a metric space. Assume that $\inf_X F_\varepsilon = \inf_K F_\varepsilon$ for some compact set $K \subset X$. Then, there holds $\lim_{\varepsilon\to 0} \inf_X F_\varepsilon = \inf_X F$. Furthermore, for any sequence x_ε in X converging to $x \in X$ with $F_\varepsilon(x_\varepsilon) = \inf_X F_\varepsilon$ we have $F(x) = \inf_X F$.*

If $F = \Gamma\text{-}\lim_{j\to\infty} F_j$ and $u \in X$, a sequence (u_j), for which the lim sup-inequality holds, is called a *recovery sequence* for u, and there clearly holds $\lim F_j(u_j) = F(u)$. It is actually the case that a sequence of minimizers is a recovery sequence for the minimizer of the Γ-limit. For this reason knowing the recovery sequences provides lots of information about the structure of the limit behaviour of the functional sequence.

For more details on the concept of Γ-convergence we refer to [35] and [53].

2.4 Functions of Bounded Variation

In the following we describe the concept and some essential results of functions of bounded variations. For an extensive monograph on this topic we refer to [10]. A more basic introduction can be found in [61].

Let $\Omega \subset \mathbb{R}^n$ be open for the rest of this section. The set of functions of bounded variation, in short $\mathrm{BV}(\Omega)$, contains all functions $u \in L^1(\Omega)$ whose distributional derivative is a Radon measure, denoted by $\mathrm{D}u$, i.e. there holds

$$\int_\Omega u \operatorname{div} w \,\mathrm{d}x = -\int_\Omega w \,\mathrm{dD}u \quad \text{for all } w \in C_c^1(\Omega;\mathbb{R}^n)\,. \tag{2.2}$$

Defining the total variation

$$\operatorname{Var}(u,\Omega) = \sup\left\{ \int_\Omega u \operatorname{div} w \,\mathrm{d}x \colon w \in C_c^1(\Omega;\mathbb{R}^n),\, \|w\|_\infty \le 1 \right\} \tag{2.3}$$

we obtain from the Riesz representation theorem that (2.2) is equivalent to the fact that $V(u,\Omega) < \infty$. Furthermore, there holds $|\mathrm{D}u|(\Omega) = V(u,\Omega)$ for all $u \in \mathrm{BV}(\Omega)$.

For any measurable function $u \colon \Omega \to \mathbb{R}$ we define for all $x \in \Omega$ the upper and lower approximate limit, respectively, by

$$u^+(x) = \inf\left\{ t \in \mathbb{R} \colon \lim_{\rho\to 0} \frac{\mathcal{L}^n\big(\{u > t\} \cap B_\rho(x)\big)}{\rho^n} = 0 \right\},$$
$$u^-(x) = \sup\left\{ t \in \mathbb{R} \colon \lim_{\rho\to 0} \frac{\mathcal{L}^n\big(\{u < t\} \cap B_\rho(x)\big)}{\rho^n} = 0 \right\}.$$

For all $x \in \Omega$ there obviously holds $u^-(x) \le u^+(x)$. If $u^-(x) = u^+(x)$ we write for their common value $u^*(x)$. The set S_u is the discontinuity set containing all those points $x \in \Omega$ for which there holds $u^-(x) < u^+(x)$.

In a similar way we can also define a notion of differentiability for measurable functions. A measurable function $u \colon \Omega \to \mathbb{R}$ is said to be *approximately differentiable* at $x \in \Omega$

if there exists a linear map, denoted by $\nabla u(x)\colon \mathbb{R}^n \to \mathbb{R}$, such that for all $\varepsilon > 0$ there holds

$$\lim_{\rho\to 0} \frac{1}{\rho^n}\,\mathcal{L}^n\left(\left\{y \in \Omega\setminus\{x\}\colon \frac{|u(y)-u^*(x)-\nabla u(x)\cdot(y-x)|}{|x-y|} > \varepsilon\right\} \cap B_\rho(x)\right) = 0\,.$$

In this way we can define the map $\nabla u\colon \Omega \to \mathbb{R}^n$, which we call the *approximate gradient* of u.

In what follows let $u \in \mathrm{BV}(\Omega)$. Then, S_u has Lebesgue measure zero and for $\mathcal{H}^{n-1}$-almost all points $x \in S_u$ one can find a unit normal vector $\nu_u(x)$ such that $u^+(x) = \left(u|_{H^+(x)}\right)^*(x)$ and $u^-(x) = \left(u|_{H^-(x)}\right)^*(x)$ with

$$\begin{aligned} H^+(x) &= \{y \in \Omega\colon \langle y-x, \nu_u(x)\rangle > 0\} \\ H^-(x) &= \{y \in \Omega\colon \langle y-x, \nu_u(x)\rangle < 0\}\,. \end{aligned}$$

If this is the case one says that x is a jump point.

We call $\tilde{u}$ a *precise representative* of u if $\tilde{u}(x) = u^*(x)$ for all $x \in \Omega\setminus S_u$ and $\tilde{u}(x) = \frac{1}{2}(u^+(x)+u^-(x))$ for all jump points $x \in S_u$. For functions of bounded variation on the real line we actually have that every point in S_u is a jump point. Furthermore, on an open interval the pointwise variation of $\tilde{u}$ and the variation as defined in (2.3) coincide. Precisely, for $a < b$ and $u \in \mathrm{BV}(a,b)$ there holds

$$\mathrm{Var}\big(u,(a,b)\big) = \sup\left\{\sum_{i=1}^N \big|\tilde{u}(t_i)-\tilde{u}(t_{i-1})\big|\colon N \in \mathbb{N}, a < t_0 < \cdots < t_N < b\right\}. \tag{2.4}$$

For any $u \in \mathrm{BV}(\Omega)$ one can split the measure $\mathrm{D}u$ in the following way

$$\mathrm{D}u = \nabla u\mathcal{L}^n + (u^+ - u^-)\cdot\nu_u\mathcal{H}^{n-1}\llcorner S_u + \mathrm{D}^c u\,,$$

where the first term, which we will denote by $\mathrm{D}^a u$, is the absolutely continuous part of $\mathrm{D}u$ with respect to the Lebesgue measure. One can show that the approximate gradient ∇u is indeed the its density function. The second term represents the jump part of u, also referred to as $\mathrm{D}^j u$, and $\mathrm{D}^c u$ is the Cantor part.

There also holds a chain rule for the composition of a Lipschitz functions and some function of bounded variation (see [10, Theorem 3.99]). Precisely, for Ω being bounded and $f\colon \mathbb{R}\to\mathbb{R}$ being Lipschitz we get that $f\circ u \in \mathrm{BV}(\Omega)$ and

$$\mathrm{D}(f\circ u) = f'(u)\nabla u\mathcal{L}^n + \big(f(u^+) - f(u^-)\big)\nu_u\mathcal{H}^{n-1}\llcorner S_u + f'(\tilde{u})\mathrm{D}^c u\,. \tag{2.5}$$

Note that f' exists almost everywhere, which follows from Rademacher's theorem.

The set of *special functions of bounded variation*, denoted by $\mathrm{SBV}(\Omega)$, contains those functions of bounded variation whose cantor part is zero, i.e. we have $\mathrm{SBV}(\Omega) = \{u \in \mathrm{BV}(\Omega) : \mathrm{D}^c u = 0\}$. The discontinuous part of such functions is therefore only concentrated on the jump set.

A measurable function $u\colon \Omega \to \mathbb{R}$ is a *generalized special function of bounded variation*, where we write $u \in \mathrm{GSBV}(\Omega)$, if any truncation of u is locally a special function of bounded variation, i.e. $u^M \in \mathrm{SBV}_{\mathrm{loc}}(\Omega)$ for all $M > 0$, with $u^M = (-M) \vee u \wedge M$. Note that for $u \in \mathrm{GSBV}(\Omega)$ the approximate gradient ∇u is defined, however, there is generally no connection to some density function of some distributional derivative. This is simply due to the fact that the distributional derivative does not need to be a measure on that space. Nevertheless, since $u^M \in \mathrm{BV}(\Omega)$, we have that $\mathrm{D}u^M$ is a measure and ∇u^M is the density function of D^{a}. One can show that $\nabla u^M(x) \to \nabla u(x)$ as $M \to \infty$ for a.a. $x \in \Omega$. Furthermore, it is well-known that $S_u = \bigcup_{M>0} S_{u^M}$. These results and more details can be found in [10, Section 4.5] and the references therein.

Moreover, we will use the following two subspaces of $\mathrm{GSBV}(\Omega)$ and $\mathrm{SBV}(\Omega)$

$$\mathrm{SBV}^2(\Omega) = \left\{u \in \mathrm{SBV}(\Omega)\colon \nabla u \in L^2(\Omega), \mathcal{H}^{n-1}(S_u) < \infty\right\}$$
$$\mathrm{GSBV}^2(\Omega) = \left\{u \in \mathrm{GSBV}(\Omega)\colon \nabla u \in L^2(\Omega), \mathcal{H}^{n-1}(S_u) < \infty\right\}.$$

Many times it is difficult to show some Γ-lim sup-inequality directly on the whole domain of the given functional. In this case one usually simplifies the problem by showing the inequality on a appropriate subset. If this set is dense in the functional domain and the functional is continuous on this dense set, one easily obtains the Γ-lim sup-inequality on the complete functional domain. One of the first density results for the Mumford-Shah functional can be found in [51]. A more general one was shown in [52, Theorem 3.1] which yields together with the therein following remarks the subsequent theorem.

Theorem 2.4.1. *Let $\Omega \subset \mathbb{R}^n$ be open and bounded with Lipschitz boundary, and take $u \in \mathrm{SBV}^2(\Omega) \cap L^\infty(\Omega)$. Then, there exists a sequence (u_j) in $\mathrm{SBV}^2(\Omega)$ such that*

(a) $\overline{S_{u_j}}$ is the intersection of Ω with a finite number of pairwise disjoint $(n-1)$-simplexes,

(b) $\mathcal{H}^{n-1}(\overline{S_{u_j}} \setminus S_{u_j}) = 0$,

(c) $u_j \in W^{k,\infty}(\Omega \setminus \overline{S_{u_j}})$ for all $k \in \mathbb{N}$,

(d) $u_j \to u$ in $L^1(\Omega)$ as $j \to \infty$,

(e) $\nabla u_j \to \nabla u$ in $L^2(\Omega;\mathbb{R}^n)$ as $j \to \infty$,

(f) $\mathcal{H}^{n-1}(S_{u_j}) \to \mathcal{H}^{n-1}(S_u)$ as $j \to \infty$.

We can replace (f) by

(g) $$\lim_{j\to\infty} \int_{S_{u_j}} \varphi(\nu_{u_j}, x) \,\mathrm{d}\mathcal{H}^{n-1} = \int_{S_u} \varphi(\nu_u, x) \,\mathrm{d}\mathcal{H}^{n-1}$$

for $\varphi(\cdot, x)$ being a norm on $\mathbb{R}^n$ for all $x \in \Omega$ and .

We now shortly introduce the concept of slicing, which is essential for the proof of the lim inf-inequality. For that let $\Omega \subset \mathbb{R}^n$ be open and bounded and let $\xi \in \mathbb{S}^{n-1}$ be a unique normal vector. Then, we write Ω_ξ for the projection of Ω onto $\xi^\perp$, and we set

$$\Omega_y^\xi := \{t \in \mathbb{R} \colon y + t\xi \subset \Omega\} \quad \text{for all } y \in \Omega_\xi \,.$$

Furthermore, for any function $u \in L^1(\Omega)$ and for $\mathcal{L}^{n-1}$-a.a. $y \in \Omega_\xi$ we can define $u_y^\xi(t) := u(y + t\xi)$ for a.a. $t \in \Omega_y^\xi$.

One can show the following important results showing the connection between a function $u \in \mathrm{SBV}(\Omega)$ and its sliced functions u_y^ξ. There are more general results for BV-functions, which are not needed in this context. The interested reader can find the details in [10, Section 3.11].

Theorem 2.4.2. *Let $u \in L^1(\Omega)$. Then $u \in \mathrm{SBV}(\Omega)$ if and only if for all $\xi \in \mathbb{S}^{n-1}$ there holds $u_y^\xi \in \mathrm{SBV}(\Omega_y^\xi)$ for $\mathcal{H}^{n-1}$-a.a. $y \in \Omega_\xi$ and*

$$\int_{\Omega_\xi} |\mathrm{D}u_y^\xi|(\Omega_y^\xi) \mathrm{d}\mathcal{L}^{n-1}(y) < \infty \,.$$

Furthermore, if $u \in \mathrm{BV}(\Omega)$ there holds for all $\xi \in \mathbb{S}^{n-1}$, for $\mathcal{H}^{n-1}$-a.a. $y \in \Omega_\xi$ and for a.a. $t \in \Omega_y^\xi$

(a) $(u_y^\xi)'(t) = \langle \nabla u(y + t\xi), \xi \rangle$,

(b) $S_{u_y^\xi} = (S_u)_y^\xi$,

(c) $(u_y^\xi)^\pm\,(t) = u^\pm(y + t\xi)$,

(d) $|\langle \mathrm{D}^* u, \xi \rangle|(\Omega) = \int_{\Omega_\xi} |\mathrm{D}^* u_y^\xi|(\Omega_y^\xi)\, \mathrm{d}\mathcal{H}^{n-1}(y) \quad$ *for* $* = a, j, c$.

The following Corollary directly follows by a truncation argument. It also directly follows from [10, Proposition 4.35].

Corollary 2.4.3. *Let $u \colon \omega \to \mathbb{R}$ be a measurable function. Then $u \in \mathrm{GSBV}(\Omega)$ if and only if for all $\xi \in \mathbb{S}^{n-1}$ there holds $u_y^\xi \in \mathrm{SBV}(\Omega_y^\xi)$ for $\mathcal{H}^{n-1}$-a.e. $y \in \Omega_\xi$ and*

$$\int_{\Omega_\xi} \big|\mathrm{D}\big((-M) \vee u_y^\xi \wedge M\big)\big|(\Omega_y^\xi) \mathrm{d}\mathcal{H}^{n-1}(y) < \infty \quad \textit{for all } M > 0 \,.$$

3 Brittle Fracture Model of Thin Elastic Shells

In this chapter we aim to develop a two-dimensional model of brittle fracture for thin elastic shells. In elasticity theory finding two-dimensional models for plates and shells has a long history, which goes back more than one hundred years with contributions from J. Bernoulli, L. Euler, G. R. Kirchhoff, T. von Kármán and many others. Some famous works are for instance the Kirchhoff-Love plate theory and the Föppl-von-Kármán equations (see [64, 84, 86, 90]).

In rigorous analysis one considers the three-dimensional "real world" model of a two dimensional surface applied with a thickness and computes the limit as the thickness tends to zero. In modern works the limit is considered in terms of Γ-convergence considering the variational formulation of the problems. In the context of elasticity theory the energy of interest is

$$\int_\Omega f(\boldsymbol{\epsilon}(u))\,\mathrm{d}x + \textit{"applied forces"}$$

for some domain $\Omega \subset \mathbb{R}^3$ and functions u describing the displacement of Ω. The function f describes the elasticity density, which depends on the underlying model.

In the case of linearized elasticity f has the form $\boldsymbol{C}\boldsymbol{\epsilon}(u) : \boldsymbol{\epsilon}(u)$ where $\boldsymbol{C}$ is the stiffness tensor and the strain $\boldsymbol{\epsilon}(u)$ is given by the symmetric gradient of the displacement u (see e.g. [47]). In this setting a quite complete work about two-dimensional models has been written by P. G. Ciarlet in [48] for Ω being a thin plate and in [49] for Ω being a thin surface. In these monographs the convergence of the solutions to the three-dimensional model is directly considered avoiding the notion of Γ-convergence. However, the results have been justified in [73] using Γ-convergence.

In the case of non-linear elasticity we find a very extensive and probably the most recent results for the planar setting in [72]. Some work for shells is for instance [71].

For now we have been talking enough about elasticity theory, and we move on to our actual topic, the brittle fracture modelling of some full elastic object. The objective three-dimensional energy functional is thus given by

$$\int_\Omega f(\boldsymbol{\epsilon}(u))\,\mathrm{d}x + \kappa\mathcal{H}^2(J_u)$$

for some domain $\Omega \subset \mathbb{R}^3$, the displacement u and some fracture set $J_u \subset \Omega$ which is the jump set of u. The function f is again the elastic energy density and $\kappa > 0$ is the toughness of the material. Note, that in this setting the minimization is performed with respect to some boundary conditions on u and there is no term of applied forces present for reasons discussed in Chapter 1.

Considering the energy density f as a function of the strain of u the right domain for the energy functional is $\mathrm{SBD}(\Omega)$ or $\mathrm{GSBD}(\Omega)$, the space of (generalized) functions of bounded deformation (for details on these spaces see [9, 54]). In this setting and under the condition of linearized elasticity we can find some dimension reduction result in [20], where the authors actually investigate thin films bonded to a stiff substrate. On the other hand density function can also be considered as a function depending on the (approximate) gradient only, meaning that the domain of the energy functional simplifies to $\mathrm{SBV}(\Omega)$ or $\mathrm{GSBV}(\Omega)$. These approaches have been used earlier in [18, 19, 33]. All the results of the cited sources here are obtained for a planar setting.

Our contribution to this topic is now the investigation of arbitrary thin shells, where we assume linearized strain and restrict the admissible displacement field to be normal to the surface. The restriction to the displacements are made in analogy with the anti-plane shear, which has been the first tackled setting in the variational formulation of fracture. The advantage of this setting is that the displacement field can be described by a scalar function, which is simply its norm, since the direction is fixed. Therefore, we can stay in the space $\mathrm{SBV}(\Omega)$.

In our strategy we consider in Section 3.2 a two-dimensional surface in $\mathbb{R}^3$, which we endow with a thickness, and we express the three-dimensional energy with respect to the curvilinear coordinates, where we first stay in the strong space $C^1(\Omega \setminus K)$. In this way the integration domain has the form $\omega \times (-\frac{\rho}{2}, \frac{\rho}{2})$, where ρ is the thickness of the surface. In a second change of variables we rescale the third coordinate, such that the integration domain becomes independent of the thickness. Then we restrict the admissible displacements to those which are normal to the surface. Only now, the functional is relaxed to $\mathrm{SBV}(\Omega)$ and, as usual, rescaled by $\frac{1}{\rho}$. Section 3.3 is then devoted to the Γ-convergence result and proof as the thickness tends to zero.

Note, that the order of coordinate transformation and relaxation must be chosen with care. Relaxing the functional before restricting it to normal displacements, would mean to consider the energy on $\mathrm{GSBD}(\Omega)$. However, this space is in general not invariant under coordinate transformation, not even under simple translations. Studying the transformation behaviour of $\mathrm{BD}(\Omega)$, $\mathrm{SBD}(\Omega)$ and $\mathrm{GSBD}(\Omega)$ arises as one of the future tasks from this chapter. For the same reason, it is not clear to which weakened function space one needs to relax the energy, if one wants to study the limit without the restriction to normal displacements.

Another technical difficulty, when studying dimension reduction for the full vectorial displacement field, is that one has to distinguish between different types of shells. From the elasticity theory we know that one obtains three different models depending on whether the surface is elliptic and on some boundary conditions (see e.g. [49]).

The content of this chapter was developed with the support of Stefano Almi. Together with the content of Chapter 6, it is planed to be published in the future in [4].

3.1 Notational Convention

In the sequel of this chapter we work only in dimension 2 and 3. We use the Einstein summing convention, i.e. in a term it is automatically summed over repeated indices without writing the sum explicitly. Furthermore, we follow the convention that Greek indices, like $\alpha, \beta, \sigma, \tau$, always run from 1 to 2, whereas Latin indices, like i, j, k, l, run form 1, to 3. Also statements where single indices are involved are meant to hold for all indices in $\{1, 2\}$ respectively $\{1, 2, 3\}$.

3.2 Geometric Setting

We assume that there exists $\omega \subset \mathbb{R}^2$ open and bounded such that the surface S is given by the image $\phi(\omega)$ of a bijective, continuous differentiable mapping $\phi\colon \omega \to \mathbb{R}^3$, of which the smooth extension to $\bar{\omega}$ is still bijective. We define the vectors $a_1 := \partial_1\phi$ and $a_2 := \partial_2\phi$ and assume that their smooth extension to $\bar{\omega}$ are (pointwise) linearly independent and, therefore, build a covariant basis. We extend these two vectors to a basis of $\mathbb{R}^3$ by the vector field a_3 normal to the surface $\phi(\omega)$, namely we set $a_3 := \frac{a_1 \times a_2}{\|a_1 \times a_2\|}$. The contravariant basis (a^i) is then defined by $a^i \cdot a_j = \delta^i_j$, where δ^i_j denotes the Kronecker delta. Note, that in the given situation there holds $a_3 = a^3$. The covariant components of the metric tensor are then given by $a_{\alpha\beta} = a_\alpha \cdot a_\beta$ and we set $(a^{\alpha\beta}) = (a_{\alpha\beta})^{-1}$. Note that there holds $a^{\alpha\beta} = a^\alpha \cdot a^\beta$.

The curvature tensor with its covariant components $b_{\alpha\beta}$, its mixed components b^β_α, and the Christoffel symbols $\Gamma^\sigma_{\alpha\beta}$ is respectively defined by

$$b_{\alpha\beta} := a_3 \cdot \partial_\alpha a_\beta\,, \qquad b^\alpha_\beta := a^{\alpha\sigma} b_{\sigma\beta}\,, \qquad \Gamma^\sigma_{\alpha\beta} := a^\sigma \cdot \partial_\alpha a_\beta\,. \tag{3.1}$$

We remark that clearly all the defined vectors and tensors depend on $x \in \omega$. However, for a better readability, this dependency will not be written explicitly.

Remark 3.2.1. The assumptions on the extensions of ϕ, and a_1 and a_2 to $\bar{\omega}$ mean that ϕ is an immersion. In this way we obtain that the metric tensor is uniformly positive definite and uniformly bounded from above, i.e. there exists some positive constants c and C, both independent of $x \in \omega$, such that

$$c|\zeta|^2 < a_{\alpha\beta}\zeta^\alpha\zeta^\beta < C|\zeta|^2 \quad \text{for all } \zeta \in \mathbb{R}^2\,. \tag{3.2}$$

Indeed, by definition we have $a_{\alpha\beta} = \nabla\phi^\top\nabla\phi$, and thus $a_{\alpha\beta}$ is positive definite on ω, i.e there holds

$$0 < a_{\alpha\beta}(x)\zeta^\alpha\zeta^\beta \quad \text{for all } \zeta \in \mathbb{R}^2, \zeta \neq 0, x \in \omega\,.$$

Using now that the extension of the right hand side is continuous with respect to x and ζ on the compact sets $\bar{\omega}$ and $\{\zeta \in \mathbb{R}^2 : |\zeta| = 1\}$, respectively, we obtain that there exist constants $c, C > 0$, not depending on $x \in \omega$, such that

$$c < a_{\alpha\beta}\zeta^\alpha\zeta^\beta < C \quad \text{for all } \zeta \in \mathbb{R}^2, |\zeta| = 1\,.$$

By a simple scaling argument we get (3.2), which clearly also holds for $(a^{\alpha\beta})$.

We regularly make use of the continuity of ϕ on the compact set $\bar{\omega}$ in order to obtain upper and lower bounds for all the defined tensor components from (3.1) as well as the upcoming ones.

Note that $\phi(\bar{\omega})$ is a manifold with boundary, whereas $\phi(\omega)$ is a manifold without boundary. If one wants to study for instance compact manifolds, such as the sphere or the torus, one would need to use more than one parametrization, each of them satisfying (3.2), and to glue them together in the right way.

We now extend the surface $\phi(\omega)$ by a thickness in the following way. Let $\rho > 0$, $\Omega_\rho = \omega \times \left(-\frac{\rho}{2}, \frac{\rho}{2}\right)$ and define $\Phi\colon \Omega_\rho \to \mathbb{R}^3$ by

$$\Phi(x) := \phi(x_1, x_2) + x_3 a_3 \quad \text{for all } x = (x_1, x_2, x_3) \in \Omega_\rho \,.$$

In the following we assume that Φ is a diffeomorphism, which is always the case for sufficiently small ρ (see [49, Theorem 3.1-1]). In the given setting there holds $\phi(\omega) = \Phi(\omega \times \{0\})$, in other words $\phi(\omega)$ is the middle surface of $\Phi(\Omega_\rho)$.

We fix some more notational conventions. In general we follow the idea that symbols with a hat on top are related to the original Cartesian coordinate system in $\Phi(\Omega_\rho)$ and the symbol without the hat to the curvilinear coordinates in Ω_ρ. Whenever x and $\hat{x}$ are used in a statement we mean $x \in \Omega_\rho$ with $\hat{x} = \Phi(x)$ and similarly for y and $\hat{y}$. We denote the coordinates of a point $x \in \Omega_\rho$ by (x_1, x_2, x_3).

For the “thick surface” $\Phi(\Omega_\rho)$ we define the covariant basis $g_i := \partial_i \Phi$ and the corresponding metric tensor $g_{ij} := g_i \cdot g_j$. By the definition of Φ we directly get

$$g_\alpha = a_\alpha + x_3 \partial_\alpha a_3 \quad \text{and} \quad g_3 = a_3 = a^3 = g^3 \,. \tag{3.3}$$

The contravariant basis (g^i) is the standard dual basis of the covariant one, i.e. it is defined by $g_i \cdot g^j = \delta_i^j$. It is easy to see that the inverse of (g_{ij}) is given by $g^{ij} := g^i \cdot g^j$.

Also for the mapping Φ we will need the corresponding Christoffel symbols, which we denote by $\Lambda_{ij}^k := g^k \cdot \partial_i g_j$. Note that there holds the symmetry $\Lambda_{ij}^k = \Lambda_{ji}^k$, which is due to $\partial_i g_j = \partial_{ij}\Phi = \partial_{ji}\Phi = \partial_j g_i$.

In the original Cartesian coordinates the energy functional with a linear elastic energy density and the crack energy, that is proportional to its surface area, is given by

$$E(\hat{u}, \hat{K}_\rho) := \frac{1}{2} \int_{\Phi(\Omega_\rho)\setminus \hat{K}_\rho} \hat{\boldsymbol{C}}^{ijkl} \hat{\boldsymbol{\epsilon}}_{ij}(\hat{u}) \hat{\boldsymbol{\epsilon}}_{kl}(\hat{u}) \,\mathrm{d}\hat{x} + \kappa \mathcal{H}^2(\hat{K}_\rho) \,, \tag{3.4}$$

for $\hat{u} \in C^1(\Phi(\Omega_\rho \setminus K_\rho); \mathbb{R}^3)$ describing the displacement field and for $\hat{K}_\rho = \Phi(K_\rho) \subset \Phi(\Omega_\rho)$ being a closed, rectifiable set describing the fracture. The stiffness tensor $\hat{\boldsymbol{C}}$ is given by

$$\hat{\boldsymbol{C}}^{ijkl} = \lambda \delta^{ij} \delta^{kl} + \mu(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk})$$

with Lamé coefficients λ and μ, where we assume that $\lambda \geq 0$ and $\mu > 0$. Furthermore, $\hat{\boldsymbol{\epsilon}}(\hat{u})$ denotes the strain given by the symmetric gradient, i.e.

$$\hat{\boldsymbol{\epsilon}}(\hat{u}) := \frac{1}{2}\left(\nabla \hat{u} + (\nabla \hat{u})^\top\right) \quad \text{or in index notation} \quad \hat{\boldsymbol{\epsilon}}_{ij}(\hat{u}) := \frac{1}{2}\left(\partial_i \hat{u}_j + \partial_j \hat{u}_i\right) . \tag{3.5}$$

The stress is given by $\hat{\boldsymbol{\sigma}}(\hat{u}) := \hat{\boldsymbol{C}}\hat{\boldsymbol{\epsilon}}(\hat{u})$, or in index notation $\hat{\boldsymbol{\sigma}}^{ij}(\hat{u}) = \hat{\boldsymbol{C}}^{ijkl}\hat{\boldsymbol{\epsilon}}(\hat{u})_{kl}$.

We now want to describe this energy functional in terms of the curvilinear coordinates. Furthermore the vector field $\hat{u}$ shall be expressed with respect to the covariant basis (g_i). Therefore, we define $u_i \colon \Omega_\rho \to \mathbb{R}$ such that

$$\hat{u}(\hat{x}) = u_i(x)g^i \quad \text{and} \quad u_j(x) = \hat{u}(\hat{x}) \cdot g_j \quad \text{for all } \hat{x} = \Phi(x), x \in \Omega_\rho\,. \tag{3.6}$$

We can express the stiffness tensor and the stress tensor in terms of the covariant basis such that they can be applied to the vector field $u = (u_1, u_2, u_3)$. In fact, there holds the following proposition.

Proposition 3.2.2. *Let* $\hat{u} \in C^1(\Phi(\Omega_\rho); \mathbb{R}^3)$ *and* $u \in C^1(\Omega_\rho; \mathbb{R}^3)$ *be given such that* (3.6) *holds. We define the strain with respect to curvilinear coordinates by*

$$\boldsymbol{\epsilon}_{ij}(u) := \frac{1}{2}(\partial_i u_j + \partial_i u_j) - u_k \Lambda^k_{ij}\,, \tag{3.7}$$

the elasticity tensor with respect to curvilinear coordinates by

$$\boldsymbol{C}^{ijkl} := \lambda g^{ij} g^{kl} + \mu(g^{ik}g^{jl} + g^{il}g^{jk})\,,$$

and the stress tensor with respect to curvilinear coordinates by

$$\boldsymbol{\sigma}^{ij}(u) := \boldsymbol{C}^{ijkl}\boldsymbol{\epsilon}_{kl}(u). \tag{3.8}$$

Then, there hold the symmetries

$$\boldsymbol{\epsilon}_{ij}(u) = \boldsymbol{\epsilon}_{ji}(u)\,, \quad \boldsymbol{C}^{ijkl} = \boldsymbol{C}^{klij} = \boldsymbol{C}^{jikl} \quad \textit{and} \quad \boldsymbol{\sigma}^{ij}(u) = \boldsymbol{\sigma}^{ji}(u)\,,$$

and the following relations:

$$\hat{C}^{ijkl}\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u})\hat{\boldsymbol{\epsilon}}_{kl}(\hat{u}) = C^{ijkl}\boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u) = \boldsymbol{\sigma}^{ij}(u)\boldsymbol{\epsilon}_{ij}(u)\,.$$

Proof. All the symmetries easily follow from the symmetries of the metric tensor and of the Christoffel symbols.

Recalling that $\partial_i\Phi = g_i$, from $\nabla\Phi^{-1}\nabla\Phi = \mathrm{Id}$ we infer $[g^i]_j = \partial_j\Phi^{-1}_i$, where $[g^i]_j$ denotes the j-th component of the vector g^i. Furthermore, there holds the identity $\Lambda^k_{ij} = g^k \cdot \partial_i g_j = -\partial_i g^k \cdot g_j$ following from the fact that $\partial_i(g^k g_j) = 0$. Hence, we have $\Lambda^k_{ij} g^j = -\partial_i g^k$. With this at hand we deduce from (3.6)

$$\partial_i\hat{u}_j = \partial_i([u_k g^k]_j \circ \Phi^{-1}) = ((\partial_l u_k)[g^k]_j + u_m\partial_l[g^m]_j)[g^l]_i = (\partial_l u_k - u_m\Lambda^m_{lk})[g^k]_j[g^l]_i\,.$$

Plugging this into (3.5) yields

$$\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u}) = \frac{1}{2}(\partial_l u_k + \partial_k u_l - 2u_m\Lambda^m_{lk})[g^k]_j[g^l]_i = \boldsymbol{\epsilon}_{kl}(u)[g^k]_j[g^l]_i\,.$$

Here, we used the symmetry of the Christoffel symbols, which leads also to the symmetry of the new defined strains, i.e. $\boldsymbol{\epsilon}_{ij}(u) = \boldsymbol{\epsilon}_{ji}(u)$.

We continue with the following simple calculations

$$\begin{aligned}\delta^{ij}\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u}) &= \boldsymbol{\epsilon}_{ij}(u)g^{ij}\,,\\ \delta^{ik}\delta^{jl}\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u})\hat{\boldsymbol{\epsilon}}_{kl}(\hat{u}) &= \boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u)g^{ik}g^{jl}\,,\\ \delta^{il}\delta^{jk}\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u})\hat{\boldsymbol{\epsilon}}_{kl}(\hat{u}) &= \boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u)g^{il}g^{jk}\,.\end{aligned}$$

Finally, we obtain

$$\begin{aligned}\hat{C}^{ijkl}\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u})\hat{\boldsymbol{\epsilon}}_{kl}(\hat{u}) &= \big(\lambda\delta^{ij}\delta^{kl} + \mu(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk})\big)\hat{\boldsymbol{\epsilon}}_{ij}(\hat{u})\hat{\boldsymbol{\epsilon}}_{kl}(\hat{u})\\ &= \lambda g^{ij}g^{kl}\boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u) + \mu(g^{ik}g^{jl} + g^{il}g^{jk})\boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u)\\ &= C^{ijkl}\boldsymbol{\epsilon}_{ij}(u)\boldsymbol{\epsilon}_{kl}(u)\\ &= \boldsymbol{\sigma}^{ij}(u)\boldsymbol{\epsilon}_{ij}(u)\,,\end{aligned}$$

where the last step follows from definition (3.8) and the symmetry of C^{ijkl}. □

We can now transform the functional in (3.4) to curvilinear coordinates in order to express it in terms of the vector field u and the set $K_\rho \subset \Omega_\rho$. Thus, for $u \in C^1(\Omega_\rho \setminus K_\rho; \mathbb{R}^3)$ and $\hat{u} \in C^1(\Phi(\Omega_\rho \setminus K_\rho); \mathbb{R}^3)$ fulfilling the relation in (3.6) we have

$$E(\hat{u}, \hat{K}) = \frac{1}{2}\int_{\Omega_\rho\setminus K_\rho} \boldsymbol{C}\boldsymbol{\epsilon}(u) : \boldsymbol{\epsilon}(u)\sqrt{g}\,\mathrm{d}x + \kappa\int_{K_\rho}\sqrt{[\nu_{K_\rho}]_i g^{ij}[\nu_{K_\rho}]_j}\sqrt{g}\,\mathcal{H}^2(x)\,, \qquad (3.9)$$

where $g := \det(g_{ij})$ and $\nu_{K_\rho}(x)$ is the unit normal to the surface K_ρ at $x \in K_\rho$.

At this point we restrict the admissible displacements to the ones that are normal to the middle surface. Hence, we consider fields of the form $u = (0, 0, u_3)$, such that (3.6) is equivalent to $\hat{u} = u_3 g^3 = u_3 a^3$. For a shorter notation we define $\tilde{\boldsymbol{\epsilon}}(u_3) = \boldsymbol{\epsilon}(0, 0, u_3)$ for all $u_3 \in C^1(\Omega_\rho \setminus K_\rho)$.

With the following proposition, we provide some useful expressions for $\tilde{\boldsymbol{\epsilon}}_{\alpha\beta}(u_3)$.

Proposition 3.2.3. *For every $u_3 \in C^1(\Omega_\rho \setminus K_\rho)$ there holds*

$$\tilde{\boldsymbol{\epsilon}}_{\alpha\beta}(u_3) = -b_{\alpha\beta}u_3 + x_3 b_\alpha^\sigma b_{\sigma\beta}u_3\,, \quad \tilde{\boldsymbol{\epsilon}}_{\alpha 3}(u_3) = \frac{1}{2}\partial_\alpha u_3\,, \quad \tilde{\boldsymbol{\epsilon}}_{33}(u_3) = \partial_3 u_3\,.$$

Proof. Inserting $(0, 0, u_3)$ in (3.7) directly yields

$$\tilde{\boldsymbol{\epsilon}}_{\alpha\beta}(u_3) = -\Lambda^3_{\alpha\beta}u_3\,, \quad \tilde{\boldsymbol{\epsilon}}_{\alpha 3}(u_3) = \frac{1}{2}\partial_\alpha u_3 - u_3\Lambda^3_{\alpha 3}\,, \quad \tilde{\boldsymbol{\epsilon}}_{33}(u_3) = \partial_3 u_3 - u_3\Lambda^3_{33}\,. \qquad (3.10)$$

The next step is to proof the formulas of Weingarten, that is

$$\partial_\alpha a_3 = \partial_\alpha a^3 = -b_{\alpha\beta}a^\beta = -b_\alpha^\sigma a_\sigma\,. \qquad (3.11)$$

Since $\partial_\alpha(a^3 \cdot a_\beta) = 0$, we simply get $b_{\alpha\beta} = -\partial_\alpha a^3 \cdot a_\beta$. Additionally, we note that $\partial_\alpha a^3 \cdot a^3 = \frac{1}{2}\partial_\alpha(a^3 \cdot a^3) = 0$, so that we can write

$$\partial_\alpha a_3 = \partial_\alpha a^3 \cdot a_\beta a^\beta = -b_{\alpha\beta}a^\beta \cdot a^\sigma a_\sigma = -b_{\alpha\beta}a^{\beta\sigma}a_\sigma = -b_\alpha^\sigma a_\sigma\,.$$

Now, by the definition of the Christoffel symbols and by (3.3) we have

$$\Lambda^3_{i3} = a_3 \cdot \partial_i a_3 = \frac{1}{2}\partial_i(a_3 \cdot a_3) = 0$$

and

$$\Lambda^3_{\alpha\beta} = a^3 \cdot \partial_\alpha(a_\beta + x_3 \partial_\beta a_3) = b_{\alpha\beta} - x_3 \partial_\alpha(b_{\beta\sigma}a^\sigma) \cdot a^3 \,. \tag{3.12}$$

Using the fact that $a^\sigma \cdot a_3 = 0$, implying $\partial_\alpha a^\sigma \cdot a_3 = -a^\sigma \cdot \partial a_3$, and (3.11) we get

$$\partial_\alpha(b_{\beta\sigma}a^\sigma) \cdot a^3 = b_{\beta\sigma}\partial_\alpha a^\sigma \cdot a_3 = -b_{\beta\sigma}a^\sigma \cdot \partial_\alpha a_3 = -b_{\beta\sigma}a^\sigma \cdot b^\tau_\alpha a_\tau = -b_{\beta\sigma}b^\sigma_\alpha \,.$$

Hence, in (3.12) we obtain

$$\Lambda^3_{\alpha\beta} = b_{\alpha\beta} - x_3 b^\sigma_\alpha b_{\sigma\beta} \,,$$

and from (3.10) the assertion follows. □

Applying another coordinate transformation in (3.9) we achieve an integration domain that is independent of ρ. Namely, we use the following scaling of the third variable:

$$\pi_\rho \colon \begin{cases} \Omega \to \Omega_\rho \\ x \mapsto (x_1, x_2, \rho x_3) \end{cases} \qquad \text{with } \Omega := \Omega_1 = \omega \times \left[-\frac{1}{2}, \frac{1}{2}\right] .$$

For any closed set $K_\rho \subset \Omega_\rho$ we set $K := \pi_\rho^{-1}(K_\rho)$. All the appearing transformed functions are endowed with a subscribed ρ, i.e. we set

$$\Lambda^3_{\alpha\beta,\rho} := \Lambda^3_{\alpha\beta} \circ \pi_\rho \,, \quad g_\rho := g \circ \pi_\rho \,, \quad g^{ij}_\rho := g^{ij} \circ \pi_\rho \,. \tag{3.13}$$

For all $u \in C^1(\Omega_\rho \setminus K_\rho)$ we set $u_\rho := u \circ \pi_\rho$ as well as $\tilde{\boldsymbol{\epsilon}}_{ij,\rho}(u_\rho) := \tilde{\boldsymbol{\epsilon}}_{ij}(u) \circ \pi_\rho$. It is easy to see that there holds

$$\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho}(u_\rho) = -\Lambda^3_{\alpha\beta,\rho}u_\rho \,, \qquad \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho}(u_\rho) = \frac{1}{2}\partial_\alpha u_\rho \,, \qquad \tilde{\boldsymbol{\epsilon}}_{33,\rho}(u_\rho) = \frac{1}{\rho}\partial_3 u_\rho \,. \tag{3.14}$$

Thus, our energy functional E can be written as

$$E(\hat{u}, \hat{K}) = \frac{\rho}{2}\int_{\Omega\setminus K} \boldsymbol{C}_\rho \tilde{\boldsymbol{\epsilon}}(u_{3,\rho}) : \tilde{\boldsymbol{\epsilon}}(u_{3,\rho})\sqrt{g_\rho}\,\mathrm{d}x + \kappa\rho \int_K \sqrt{[\nu_K]_i g^{ij}_\rho [\nu_K]_j}\sqrt{g_\rho}\,\mathcal{H}^2(x) \,, \tag{3.15}$$

for all $\hat{u} = u_3 g^3$ with $u_3 \in C^1(\Omega_\rho \setminus K_\rho)$.

In order to simplify the energy even more we have a closer look on how the scaled Christoffel symbols and the scaled metric tensor depend on the thickness ρ.

Proposition 3.2.4. *For g^{ij}_ρ, g_ρ and $\Lambda^3_{\alpha\beta,\rho}$ defined as in* (3.13) *there holds*

$$g_\rho = a + O(\rho) \,,$$

$$g^{\alpha\beta}_\rho = a^{\alpha\beta} + O(\rho) \,, \qquad g^{\alpha 3}_\rho = 0 \,, \qquad g^{33}_\rho = 1 \,, \tag{3.16}$$

$$\Lambda^3_{\alpha\beta,\rho} = b_{\alpha\beta} - \rho x_3 b^\sigma_\alpha b_{\sigma\beta} = b_{\alpha\beta} + O(\rho) \,. \tag{3.17}$$

The convergence rates as $\rho \to 0$ are uniformly, i.e. they do not depend on $x \in \Omega$.

Furthermore, for $\rho > 0$ sufficiently small, the tensors with components $g_{ij,\rho} := g_{ij} \circ \pi_\rho$ and g_ρ^{ij} are uniformly positive definite and uniformly bounded from above, i.e. there exists $c, C > 0$, independent of $x \in \Omega$ and ρ, such that

$$c|\zeta|^2 \leq g_{ij,\rho}\zeta^i\zeta^j \leq C|\zeta|^2 \quad \textit{and} \quad c|\zeta|^2 \leq g_\rho^{ij}\zeta_i\zeta_j \leq C|\zeta|^2 \quad \textit{for all } \zeta \in \mathbb{R}^3 . \tag{3.18}$$

Proof. From (3.3) we simply get

$$g_{\alpha,\rho} = g_\alpha \circ \pi_\rho = a_\alpha + \rho x_3 \partial_\alpha a_3 \quad \text{and} \quad g_{3,\rho} = a_3 .$$

Thus, we can compute

$$\begin{aligned} g_{\alpha\beta,\rho} &= a_{\alpha\beta} + \rho x_3 \partial_\alpha a_3 \cdot a_\beta + \rho x_3 \partial_\alpha a_3 \cdot a_\beta + \rho^2 x_3^2 \partial_\alpha a_3 \cdot \partial_\beta a_3 \\ &= a_{\alpha\beta} - 2\rho x_3 b_{\alpha\beta} + \rho^2 x_3^2 \partial_\alpha a_3 \cdot \partial_\beta a_3 . \end{aligned}$$

Using $a_i \cdot a_3 = \delta_{i3}$ as well as $\partial_\alpha a_3 \cdot a_3 = \frac{1}{2}\partial_\alpha(a_3 \cdot a_3) = 0$ we get $g_{\alpha 3,\rho} = 0$ and $g_{33} = 1$.

Since x_3, $b_{\alpha\beta}$ and $\partial_\alpha a_3$ are bounded we get

$$g_{\alpha\beta,\rho} = a_{\alpha\beta} + O(\rho) , \quad g_{\alpha 3} = 0 \quad \text{and} \quad g_{33} = 1 ,$$

with uniform convergence with respect to ρ. The expression for g_ρ is now straight forward and for ρ sufficiently small we obtain from (3.2) the first part of (3.18). The second part then simply follows from $(g_\rho^{ij}) = (g_{ij,\rho})^{-1}$.

By Taylor's expansion we get

$$\begin{aligned} (g_\rho^{ij}) = (g_{ij,\rho})^{-1} &= \left(\begin{array}{cc|c} \multicolumn{2}{c|}{\multirow{2}{*}{$(a_{\alpha\beta})$}} & 0 \\ & & 0 \\ \hline 0 & 0 & 1 \end{array}\right)^{-1} \\ &\quad + 2\rho x_3 \left(\begin{array}{cc|c} \multicolumn{2}{c|}{(a_{\alpha\beta})} & 0 \\ & & 0 \\ \hline 0 & 0 & 1 \end{array}\right)^{-1} \left(\begin{array}{cc|c} \multicolumn{2}{c|}{(b_{\alpha\beta})} & 0 \\ & & 0 \\ \hline 0 & 0 & 0 \end{array}\right) \left(\begin{array}{cc|c} \multicolumn{2}{c|}{(a_{\alpha\beta})} & 0 \\ & & 0 \\ \hline 0 & 0 & 1 \end{array}\right)^{-1} + O(\rho^2) \end{aligned}$$

With this at hand one can simply calculate $g_\rho^i = g_\rho^{ij} g_{j,\rho}$ up to the order ρ. Since $g_{ij,\rho}$ converges uniformly, so does g_ρ^{ij} as its inverse.

The formulas (3.17) directly follow from Proposition 3.2.3. □

Using $g_\rho^{\alpha 3} = 0$ and $g_\rho^{33} = 1$ from the previous proposition in (3.15) we have shown the following: For $\hat{K}_\rho \subset \Phi(\Omega_\rho)$ closed we set $K = \pi^{-1} \circ \Phi^{-1}(\hat{K}_\rho)$. Furthermore, let $u_\rho \in C^1(\Omega \setminus K)$, $\hat{u} \in C^1(\Phi(\Omega_\rho \setminus K_\rho); \mathbb{R}^3)$ satisfying the relation $\hat{u} = u g_\rho^3$, with $u_\rho = u \circ \pi_\rho$. Then, there holds

$$E(\hat{u}, \hat{K}_\rho) = \frac{\rho}{2} \int_\Omega \boldsymbol{C}_\rho \tilde{\boldsymbol{\epsilon}}_\rho(u_\rho) \colon \tilde{\boldsymbol{\epsilon}}_\rho(u_\rho) \sqrt{g_\rho} \, \mathrm{d}x$$

$$+\,\rho\kappa\int_K\sqrt{[\nu_K]_\alpha g_\rho^{\alpha\beta}[\nu_K]_\beta+\frac{1}{\rho^2}[\nu_K]_3^2}\sqrt{g_\rho}\,\mathcal{H}^2(x)\,. \quad (3.19)$$

With the next statement we conclude these preliminaries and attend to the formulation and the proof of the main result of this chapter in the next section.

Proposition 3.2.5. *The scaled three-dimensional stiffness tensor* $\boldsymbol{C}_\rho^{ijkl}=\boldsymbol{C}^{ijkl}\circ\pi_\rho$ *is given by*

$$\boldsymbol{C}_\rho^{ijkl}=\lambda g_\rho^{ij}g_\rho^{kl}+\mu(g_\rho^{ik}g_\rho^{jl}+g_\rho^{il}g_\rho^{jk})\,, \quad (3.20)$$

with the symmetries $\boldsymbol{C}_\rho^{ijkl}=\boldsymbol{C}_\rho^{klij}=\boldsymbol{C}_\rho^{jikl}$. *Particularly, there holds*

$$\begin{aligned}
&\boldsymbol{C}_\rho^{\alpha\beta\sigma\tau}=\lambda a^{\alpha\beta}a^{\sigma\tau}+\mu(a^{\alpha\sigma}a^{\beta\tau}+a^{\alpha\tau}a^{\beta\sigma})+O(\rho)\,, && \boldsymbol{C}_\rho^{\alpha\beta\sigma3}=0\,,\\
&\boldsymbol{C}_\rho^{\alpha3\beta3}=\mu a^{\alpha\beta}+O(\rho)\,, && \boldsymbol{C}_\rho^{\alpha\beta33}=\lambda a^{\alpha\beta}+O(\rho)\,,\\
&\boldsymbol{C}_\rho^{\alpha333}=0\,, && \boldsymbol{C}_\rho^{3333}=\lambda+2\mu\,.
\end{aligned}$$

Furthermore, there exists $\rho_0>0$ *and some constants* $c,C>0$ *independent of* $x\in\Omega$ *and* ρ *such that for all* $0<\rho\le\rho_0$

$$c\|m\|_2^2\le\boldsymbol{C}_\rho^{ijkl}m_{ij}m_{kl}\le C\|m\|_2^2\quad\textit{for all }(m_{ij})\in\mathbb{R}^{3\times3}\textit{ symmetric}\,. \quad (3.21)$$

The norm $\|\cdot\|_2$ *denotes here the Frobenius norm, i.e.* $\|m\|_2^2=\sum_{i,j}|m_{ij}|^2$.

Proof. Throughout the proof, we use $c,C>0$ as generic constants, independent of $x\in\omega$ and ρ, which may vary from line to line.

The symmetries are straight forward and the expressions for $\boldsymbol{C}_\rho^{ijkl}$ follow by inserting (3.16) in (3.20).

Define

$$\begin{aligned}
&\boldsymbol{C}_0^{\alpha\beta\sigma\tau}=\lambda a^{\alpha\beta}a^{\sigma\tau}+\mu(a^{\alpha\sigma}a^{\beta\tau}+a^{\alpha\tau}a^{\beta\sigma})\,, && \boldsymbol{C}_0^{\alpha\beta\sigma3}=0\,, && \boldsymbol{C}_0^{\alpha3\beta3}=\mu a^{\alpha\beta}\,,\\
&\boldsymbol{C}_0^{\alpha\beta33}=\lambda a^{\alpha\beta}\,, && \boldsymbol{C}_0^{\alpha333}=0\,, && \boldsymbol{C}_0^{3333}=\lambda+2\mu\,.
\end{aligned}$$

We first show that

$$c\|m\|_2^2\le\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl}\le C\|m\|_2^2\quad\text{for all }m\in\mathbb{R}^{3\times3}\text{ symmetric.} \quad (3.22)$$

Indeed, for all $m\in\mathbb{R}^{3\times3}$ being symmetric we can write

$$\begin{aligned}
\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl}=\lambda(a^{\alpha\beta}m_{\alpha\beta}+m_{33})^2+\mu(a^{\alpha\sigma}a^{\beta\tau}+a^{\alpha\tau}a^{\beta\sigma})m_{\alpha\beta}m_{\sigma\tau}&\\
+\,4\mu a^{\alpha\beta}m_{\alpha3}m_{\beta3}+2\mu(m_{33})^2\,.& \quad (3.23)
\end{aligned}$$

We continue with a closer look on the single terms in (3.23). The first and last term are clearly non-negative. Also from the positive definiteness of $a^{\alpha\beta}$ (see (3.2)) we get

$$c|m_{\alpha3}|^2\le a^{\alpha\beta}m_{\alpha3}m_{\beta3}\le C|m_{\alpha3}|^2\quad\text{for all }m\in\mathbb{R}^{3\times3}\,.$$

It remains to show that the second term in (3.23) is positive. Since $a^{\alpha\beta}$ is symmetric there holds $\det(a^{\alpha\beta}) = a^{11}a^{22} - (a^{12})^2$ and we compute

$$\begin{aligned} a^{\alpha\sigma}a^{\beta\tau}m_{\alpha\beta}m_{\sigma\tau} &= (a^{11}m_{11})^2 + 4a^{11}a^{12}m_{11}m_{12} + 2(a^{11}a^{22} + (a^{12})^2)(m_{12})^2 \\ &\quad + 2(a^{12})^2 m_{11}m_{22} + 4a^{12}a^{22}m_{12}m_{22} + (a^{22}m_{22})^2 \\ &= \Big(a^{11}m_{11} + 2a^{12}m_{12} + \frac{(a^{12})^2}{a^{11}}m_{22}\Big)^2 + 2\det(a^{\alpha\beta})\Big(m_{12} + \frac{a^{12}}{a^{11}}m_{22}\Big)^2 \\ &\quad + \frac{1}{(a^{11})^2}\Big(\det(a^{\alpha\beta})^2 + 2(a^{12})^4\Big)(m_{22})^2 \,. \end{aligned}$$

From (3.2) we get

$$c \le a^{11} \le C\,, \quad \text{and} \quad c \le \det(a^{\alpha\beta}) \le C\,,$$

from which we infer

$$c \le a^{\alpha\sigma}a^{\beta\tau}m_{\alpha\beta}m_{\sigma\tau} \le C \quad \text{for all } m \in \mathbb{R}^{2\times 2} \text{ symmetric, } \|m\|_2 = 1\,.$$

Recalling that $\mu > 0$ and using a scaling argument we obtain

$$c\|m\|_2^2 \le \mu(a^{\alpha\sigma}a^{\beta\tau} + a^{\alpha\tau}a^{\beta\sigma})m_{\alpha\beta}m_{\sigma\tau} \le C\|m\|_2^2 \quad \text{for all } m \in \mathbb{R}^{2\times 2} \text{ symmetric.}$$

We have thus shown (3.22).

From the uniform convergence rate as $\rho \to 0$ (see Proposition 3.2.4), we infer that there exists some $\tilde{C} > 0$ and $\rho_0 > 0$, both independent of x such that for all $m \in \mathbb{R}^{3\times 3}$ symmetric with $\|m\|_2 = 1$

$$\frac{\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl}}{\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl} + \tilde{C}\rho_0} \le \frac{\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl}}{\boldsymbol{C}_\rho^{ijkl}m_{ij}m_{kl}} \le \frac{\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl}}{\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl} - \tilde{C}\rho_0} \quad \text{for all } 0 < \rho \le \rho_0\,.$$

Because of (3.22) we obtain a uniform upper and lower bound of the right and left hand side, respectively. Therefore, we obtain

$$c\,\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl} \le \boldsymbol{C}_\rho^{ijkl}m_{ij}m_{kl} \le C\boldsymbol{C}_0^{ijkl}m_{ij}m_{kl} \quad \text{for all } m \in \mathbb{R}^{3\times 3} \text{ symmetric}\,.$$

Using these inequalities in (3.22) we deduce the assertion. □

3.3 The Two-Dimensional Shell Model

To give a meaning to the limit for $\rho \to 0$ we need to rescale the energy in (3.19) by ρ^{-1}. Otherwise the limit would be just the zero functional. We remark that as long as $\rho > 0$ such a scaling does not change the “three-dimensional” minimizer of the functional. However, considering the limit as $\rho \to 0$ it is crucial to scale the functional in the right way, as we do here.

For the following we focus on the right hand side of (3.19) as a functional with domain $C^1(\Omega \setminus K)$ and therefore we will also omit the subscript ρ when appropriate.

Furthermore, as usual in the theory of free discontinuity problem, we relax this functional to generalized special functions of bounded variation and replace in (3.19) the set K by the discontinuity set S_{u_ρ}. Hence, for all $u \in \mathrm{GSBV}(\Omega)$ and for all $\rho > 0$ we define the energy functional

$$F_\rho(u) := \frac{1}{2}\int_\Omega \boldsymbol{C}_\rho \tilde{\boldsymbol{\epsilon}}_\rho(u) : \tilde{\boldsymbol{\epsilon}}_\rho(u)\sqrt{g_\rho}\,\mathrm{d}x \\ + \kappa \int_{S_u} \sqrt{[\nu_{S_u}]_\alpha g_\rho^{\alpha\beta}[\nu_{S_u}]_\beta + \frac{1}{\rho^2}(\nu_{S_u})_3^2}\sqrt{g_\rho}\,\mathcal{H}^2(x)\,.$$

We note that the relaxation to $\mathrm{GSBV}(\Omega)$ guarantees the existence of minimizers. This follows by the direct method of calculus of variations using the compactness property of the function space $\mathrm{GSBV}(\Omega)$ together with the lower semi-continuity of F_ρ as shown in [10] (see also [6, 7, 8]).

Our main result of this chapter is now to compute the Γ-limit of the functional F_ρ. As we aim for a two-dimensional model we expect our limit functional to be defined for functions on ω, which we will identify with functions on Ω being independent of x_3 in order to give sense to the limits. For this reason, we define the function space

$$\mathcal{U} = \{u \in \mathrm{GSBV}^2(\Omega) \mid \partial_3 u = 0, (\nu_u)_3 = 0\} \cong \mathrm{GSBV}^2(\omega)\,.$$

We stress that the conditions $\partial_3 u = 0$ and $(\nu_u)_3 = 0$ in the definition of $\mathcal{U}$ are not redundant. In fact for $u \in \mathcal{U} \cap \mathrm{SBV}^2(\Omega)$, $\partial_3 u$ is not the distributional derivative of u along the third variable but its absolutely continuous part with respect to the Lebesgue measure. Together with $(\nu_u)_3 = 0$ it follows that the third component of Du is zero and thus u is constant along the third variable. By a simple truncation argument it can be seen that every $u \in \mathcal{U}$ is constant with respect to the third variable. Therefore, the identification of $\mathcal{U}$ with $\mathrm{GSBV}^2(\omega)$ is justified.

Remark 3.3.1. Identifying $\mathcal{U}$ with $\mathrm{GSBV}^2(\omega)$ there is no difference in integrating over ω or Ω. In fact, for every $u \in \mathcal{U}$ there exists $\bar{u} \in \mathrm{GSBV}^2(\omega)$, such that $u(x_1, x_2, x_3) = \bar{u}(x_1, x_2)$ for every $(x_1, x_2, x_3) \in \Omega$. Therefore,

$$\int_\Omega u\,\mathrm{d}(x_1, x_2, x_3) = \int_{\frac{1}{2}}^{\frac{1}{2}} \int_\omega u\,\mathrm{d}(x_1, x_2)\mathrm{d}x_3 = \int_\omega \bar{u}\,\mathrm{d}(x_1, x_2)\,.$$

The same holds for the integration over $S_{\bar{u}}$ and S_u, where the former has dimension one and the latter has dimension two.

We can now present the functional, which will turn out to be the desired limit of F_ρ as $\rho \to 0$: For all $u \in \mathcal{U}$ we define

$$F_0(u) := \frac{1}{2}\int_\Omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a}\,\mathrm{d}x + \frac{\mu}{2}\int_\Omega a^{\alpha\beta}\partial_\alpha u \partial_\beta u \sqrt{a}\,\mathrm{d}x \\ + \kappa \int_{S_u} \sqrt{[\nu_u]_\alpha a^{\alpha\beta}[\nu_u]_\beta}\,\sqrt{a}\,\mathrm{d}\mathcal{H}^1$$

where we set

$$a := \det(a_{\alpha\beta}) \quad \text{and} \quad \boldsymbol{c}^{\alpha\beta\sigma\tau} := \frac{2\lambda\mu}{\lambda+2\mu} a^{\alpha\beta}a^{\sigma\tau} + \mu\big(a^{\alpha\sigma}a^{\beta\tau} + a^{\alpha\tau}a^{\beta\sigma}\big)\,.$$

In virtue of Remark 3.3.1 we can define F_0 also on $\mathrm{GSBV}^2(\omega)$ and integrate over ω.

Remark 3.3.2. In the same way as we have shown (3.22), we get that there exists $c, C > 0$ with

$$c\|m\|_2 \leq c^{\alpha\beta\sigma\tau} m_{\alpha\beta} m_{\sigma\tau} \leq C\|m\|_2 \quad \text{for all } m \in \mathbb{R}^{2\times 2} \text{ symmetric.}$$

This implies that $F_0(u) < \infty$ is equivalent to $(b_{\alpha\beta})u \in L^2(\Omega;\mathbb{R}^{2\times 2})$.

We are now ready to state the result describing the two dimensional model in terms of a Γ-convergence argument as the thickness ρ tends to zero.

Theorem 3.3.3. *Define the functional* $\mathcal{F}_\rho \colon L^1(\Omega) \to \mathbb{R}$ *by*

$$\mathcal{F}_\rho(u) = \begin{cases} F_\rho(u) & \text{for } u \in \mathrm{GSBV}^2(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

and $\mathcal{F}_0 \colon L^1(\Omega) \to \mathbb{R}$ *by*

$$\mathcal{F}_0(u) = \begin{cases} F_0(u) & \text{for } u \in \mathcal{U} \\ +\infty & \text{otherwise}\,. \end{cases}$$

Then $\mathcal{F}_\rho$ Γ*-converges to* $\mathcal{F}$ *as* $\rho \to 0$.

The proof of Theorem 3.3.3 is split in the usual two steps of firstly showing the lim inf-inequality in Proposition 3.3.5 and secondly showing the lim sup-inequality in Proposition 3.3.6. But first of all we show an auxiliary result.

Lemma 3.3.4. *Let* $\rho_n > 0$ *be a null sequence. Let* $u_n \in L^1(\Omega)$ *for all* $n \in \mathbb{N}$ *such that* $u_n \to u$ *in* $L^1(\Omega)$ *as* $n \to \infty$ *and* $\sup_{n\in\mathbb{N}} \mathcal{F}_{\rho_n}(u_n) < \infty$. *Then* $u \in \mathcal{U}$ *and up to subsequence* $\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n) \rightharpoonup -b_{\alpha\beta}u$ *and* $\partial_\alpha u_n \rightharpoonup \partial_\alpha u$ *in* $L^2(\Omega)$. *Furthermore, there holds* $\int_{S_{u_n}} [\nu_{u_n}]_3 \, \mathrm{d}\mathcal{H}^2 \to 0$.

Proof. Throughout the proof $C > 0$ denotes a generic constant, independent of $x \in \Omega$ and $\rho_n > 0$. Since $\mathcal{F}_{\rho_n}(u_n)$ is bounded we have that $u_n \in \mathrm{GSBV}^2(\Omega)$.

From (3.14) we simply get for sufficiently small ρ_n

$$\begin{aligned} |\nabla u_n|^2 &= \sum_\alpha |2\tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n)|^2 + |\rho_n \tilde{\boldsymbol{\epsilon}}_{33,\rho_n}(u_n)|^2 \\ &\leq 4\sum_{i,j} |\tilde{\boldsymbol{\epsilon}}_{ij,\rho_n}(u_n)|^2 \\ &\leq C \boldsymbol{C}^{ijkl}_{\rho_n} \tilde{\boldsymbol{\epsilon}}_{ij,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{kl,\rho_n}(u_n)\,, \end{aligned} \tag{3.24}$$

where the last inequality follows from (3.21).

Furthermore, from Proposition 3.2.4 we can infer that

$$C \leq [\nu_{u_n}]_\alpha g^{\alpha\beta}_{\rho_n} [\nu_{u_n}]_\beta + \frac{1}{\rho_n^2}\big([\nu_{u_n}]_3\big)^2 \quad \text{and} \quad C \leq g_{\rho_n} \,. \tag{3.25}$$

In consequence there holds

$$C\bigg(\int_\Omega |\nabla u_n|^2 \,\mathrm{d}x + \mathcal{H}^2(S_{u_n})\bigg) \leq \mathcal{F}_{\rho_n}(u_n)\,,$$

where the right hand side is uniformly bounded in view of the assumption. Because of the L^1-convergence of u_n, $\|u_n\|_{L^1}$ is uniformly bounded, and thus, by compactness properties of $\mathrm{GSBV}(\Omega)$ (see e.g. [10, Theorem 4.36]) there holds $u \in \mathrm{GSBV}^2(\Omega)$ and $\nabla u_n \rightharpoonup \nabla u$ in $L^2(\Omega;\mathbb{R}^n)$. Applying for instance [10, Theorem 5.8] we get

$$\int_\Omega |\partial_3 u|^2 \,\mathrm{d}x \leq \liminf_{n\to\infty} \int_\Omega |\partial_3 u_n|^2 \,\mathrm{d}x\,,$$

and hence, we can compute, using (3.14) and the second half of (3.24)

$$\int_\Omega |\partial_3 u|^2 \,\mathrm{d}x \leq \liminf_{n\to\infty} \rho_n^2 \int_\Omega \big|\tilde{\epsilon}_{33,\rho_n}(u_n)\big|^2 \,\mathrm{d}x \leq C \liminf_{n\to\infty} \rho_n \mathcal{F}_{\rho_n}(u_n) \to 0\,,$$

as $n \to \infty$, which yields $\partial_3 u = 0$.

Next, we show that $[\nu_u]_3 = 0$. From [10, Theorem 5.22] we obtain the following lower semi-continuity property: For every $\tilde{\rho} > 0$ there holds

$$\begin{aligned}\int_{S_u} &\sqrt{[\nu_u]_\alpha a^{\alpha\beta}[\nu_u]_\beta + \frac{1}{\tilde{\rho}^2}\big|[\nu_u]_3\big|^2}\sqrt{a}\,\mathrm{d}\mathcal{H}^2(x) \\ &\leq \liminf_{n\to\infty} \int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha a^{\alpha\beta}[\nu_{u_n}]_\beta + \frac{1}{\tilde{\rho}^2}\big|[\nu_{u_n}]_3\big|^2}\sqrt{a}\,\mathrm{d}\mathcal{H}^2(x)\,. \end{aligned} \tag{3.26}$$

With this at hand we estimate for all $\tilde{\rho} > 0$

$$\begin{aligned}\int_{S_u} &\big|[\nu_u]_3\big|\sqrt{a}\,\mathrm{d}\mathcal{H}^2(x) \\ &\leq \tilde{\rho} \liminf_{n\to\infty} \int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha a^{\alpha\beta}[\nu_{u_n}]_\beta + \frac{1}{\tilde{\rho}^2}\big|[\nu_{u_n}]_3\big|^2}\sqrt{a}\,\mathrm{d}\mathcal{H}^2(x)\,. \end{aligned} \tag{3.27}$$

From Proposition 3.2.4 and (3.25) we get for sufficiently large $n \in \mathbb{N}$

$$\begin{aligned} &\int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha a^{\alpha\beta}[\nu_{u_n}]_\beta + \frac{1}{\tilde{\rho}^2}\big|[\nu_{u_n}]_3\big|^2}\sqrt{a}\,\mathrm{d}\mathcal{H}^2(x) \\ \leq &\int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha g^{\alpha\beta}_{\rho_n}[\nu_{u_n}]_\beta + \frac{1}{\rho_n^2}\big|[\nu_{u_n}]_3\big|^2}\sqrt{g_{\rho_n}}\,\mathrm{d}\mathcal{H}^2(x) \\ &+ C\sqrt{\rho_n}\int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha g^{\alpha\beta}_{\rho_n}[\nu_{u_n}]_\beta + \frac{1}{\rho_n^2}\big|[\nu_{u_n}]_3\big|^2} + \sqrt{g_{\rho_n}}\,\mathrm{d}\mathcal{H}^2(x) + C\rho_n \\ \leq &\,\mathcal{F}_{\rho_n}(u_n) + C\sqrt{\rho_n}\mathcal{F}_{\rho_n}(u_n) + C\rho_n\,. \end{aligned} \tag{3.28}$$

By assumption, the right hand side is uniformly bounded. Consequently, in (3.27) we get

$$\int_{S_u} \big|[\nu_u]_3\big| \sqrt{a} \, \mathrm{d}\mathcal{H}^2(x) \le C\sqrt{\tilde{\rho}} \quad \text{for all } \tilde{\rho} > 0 \,,$$

and we must have $[\nu_u]_3 = 0$, so that $u \in \mathcal{U}$.

As in (3.24) we get that $\|\partial_\alpha u_n\|_{L^2}$ and $\|\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho}(u_n)\|_{L^2}$ are uniformly bounded. The weak convergences then follow together with (3.14) and (3.17). □

We now show the required lim inf-inequality.

Proposition 3.3.5. *In the setting of Theorem 3.3.3 there holds* $\mathcal{F} \le \Gamma\text{-}\liminf_{\rho\to 0} \mathcal{F}_\rho$.

Proof. Let $\rho_n > 0$ be a null sequence, and let u_n be a sequence in $L^1(\Omega)$ converging to u in $L^1(\Omega)$. Without loss of generality we can assume that $\liminf_{n\to\infty} \mathcal{F}_{\rho_n}(u_n) = \lim_{n\to\infty} \mathcal{F}_{\rho_n}(u_n) < \infty$. From Lemma 3.3.4 we thus get that $u \in \mathcal{U}$.

Using (3.2.5) and completing squares in a suitable way we can write

$$F_{\rho_n}(u_n) = I^{(1)}_{\rho_n}(u_n) + I^{(2)}_{\rho_n}(u_n) + I^{(3)}_{\rho_n}(u_n) + I^{(4)}_{\rho_n}(u_n) \tag{3.29}$$

with

$$I^{(1)}_{\rho_n}(u_n) := \frac{1}{2}\int_\Omega \Big(\frac{2\lambda\mu}{\lambda+2\mu} g^{\alpha\beta}_{\rho_n} g^{\sigma\tau}_{\rho_n} + \mu\big(g^{\alpha\sigma}_{\rho_n} g^{\beta\tau}_{\rho_n} + g^{\alpha\tau}_{\rho_n} g^{\beta\sigma}_{\rho_n}\big)\Big) \tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\sigma\tau,\rho_n}(u_n) \sqrt{g_{\rho_n}} \, \mathrm{d}x$$

$$I^{(2)}_{\rho_n}(u_n) := \frac{1}{2}\int_\Omega (\lambda+2\mu)\Big(\frac{\lambda}{\lambda+2\mu} g^{\alpha\beta}_{\rho_n} \tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n) + \tilde{\boldsymbol{\epsilon}}_{33,\rho_n}(u_n)\Big)^2 \sqrt{g_{\rho_n}} \, \mathrm{d}x$$

$$I^{(3)}_{\rho_n}(u_n) := 2\mu \int_\Omega g^{\alpha\beta}_{\rho_n} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{g_{\rho_n}} \, \mathrm{d}x$$

$$I^{(4)}_{\rho_n}(u_n) := \kappa \int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha g^{\alpha\beta}_{\rho_n} [\nu_{u_n}]_\beta + \frac{1}{\rho_n^2}\big|[\nu_{u_n}]_3\big|^2} \sqrt{g_{\rho_n}} \, \mathrm{d}\mathcal{H}^2 \,.$$

We will now show the lim inf-inequality for $I^{(1)}_{\rho_n}$, $I^{(3)}_{\rho_n}$ and $I^{(4)}_{\rho_n}$. Since $I^{(2)}_{\rho_n}$ is non-negative it can be simply added at the end.

By pointwise convergences (up to subsequence) of u_n almost everywhere and by the convergence rates from Proposition 3.2.4 we get the pointwise convergence of the integrand of $I^{(1)}_{\rho_n}(u_n)$ almost everywhere. Hence, we can apply Fatou's lemma in order to get

$$\frac{1}{2}\int_\Omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a} \, \mathrm{d}x \le \liminf_{n\to\infty} I^{(1)}_{\rho_n}(u_n) \,. \tag{3.30}$$

Note that as a norm in $L^2(\omega)$ the mapping $v \mapsto \int_\omega a^{\alpha\beta} v_\alpha v_\beta \sqrt{a} \, \mathrm{d}x$ is convex and because of (3.2) also continuous, and thus, it is also weakly lower semi-continuous. Hence, using the weak convergence of $\tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \rightharpoonup \frac{1}{2}\partial_\alpha u$ in $L^2(\Omega)$ from Lemma 3.3.4, we obtain

$$\frac{1}{4}\int_\Omega a^{\alpha\beta} \partial_\alpha u \partial_\beta u \sqrt{a} \, \mathrm{d}x \le \liminf_{n\to\infty} \int_\Omega a^{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{a} \, \mathrm{d}x \,.$$

From Proposition 3.2.4 we get for sufficiently large $n \in \mathbb{N}$

$$\begin{aligned}
&\int_\Omega a^{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{a}\,\mathrm{d}x \\
\leq &\int_\Omega g_{\rho_n}^{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{g_{\rho_n}}\,\mathrm{d}x + C\sqrt{\rho_n} \int_\Omega g_{\rho_n}^{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n)\,\mathrm{d}x \\
&+ C\rho_n \int_\Omega \sum_{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{g_{\rho_n}}\,\mathrm{d}x + C\rho_n^{\frac{3}{2}} \int_\Omega \sum_{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n)\,\mathrm{d}x \\
\leq &\int_\Omega g_{\rho_n}^{\alpha\beta} \tilde{\boldsymbol{\epsilon}}_{\alpha 3,\rho_n}(u_n) \tilde{\boldsymbol{\epsilon}}_{\beta 3,\rho_n}(u_n) \sqrt{g_{\rho_n}}\,\mathrm{d}x + C\sqrt{\rho_n}\mathcal{F}_{\rho_n}(u_n)
\end{aligned}$$

As a consequence we deduce

$$\frac{\mu}{2} \int_\omega a^{\alpha\beta} \partial_\alpha u \cdot \partial_\beta u \sqrt{a}\,\mathrm{d}x \leq \liminf_{n\to\infty} I_{\rho_n}^{(3)}(u_n)\,. \tag{3.31}$$

With the lower semi-continuity property (3.26) and estimating as in (3.28) we compute for any $\tilde{\rho} > 0$

$$\begin{aligned}
&\int_{S_u} \sqrt{[\nu_u]_\alpha a^{\alpha\beta} [\nu_u]_\beta} \sqrt{a}\,\mathrm{d}\mathcal{H}^1 \\
\leq &\liminf_{n\to\infty} \int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha a^{\alpha\beta} [\nu_{u_n}]_\beta + \frac{1}{\tilde{\rho}^2} \left|[\nu_{u_n}]_3\right|^2} \sqrt{a}\,\mathrm{d}\mathcal{H}^2 \\
\leq &\liminf_{n\to\infty} \left(\int_{S_{u_n}} \sqrt{[\nu_{u_n}]_\alpha g_{\rho_n}^{\alpha\beta} [\nu_{u_n}]_\beta + \frac{1}{\rho_n^2} \left|[\nu_{u_n}]_3\right|^2} \sqrt{g_{\rho_n}}\,\mathrm{d}\mathcal{H}^2 + C\sqrt{\rho_n} \right).
\end{aligned}$$

Hence, we obtain

$$\kappa \int_{S_u} \sqrt{[\nu_u]_\alpha a^{\alpha\beta} [\nu_u]_\beta} \sqrt{a}\,\mathrm{d}\mathcal{H}^2 \leq \liminf_{n\to\infty} I_{\rho_n}^{(4)}(u_n)\,. \tag{3.32}$$

Summing up (3.30), (3.31) and (3.32), and using that $I_{\rho_n}^{(2)}$ is non-negative, we deduce that

$$\mathcal{F}(u) \leq \liminf_{n\to\infty} \mathcal{F}_{\rho_n}(u_n)\,.$$

Note that for now the inequality holds for a subsequence which we have extracted during the proof. However, since we assumed that the lim inf actually is a limit, we get the assertion for the complete sequence. □

In the next proposition we proof the lim sup-inequality.

Proposition 3.3.6. *There holds* $\Gamma\text{-}\limsup_{\rho\to 0} \mathcal{F}_\rho \leq \mathcal{F}$.

Proof. Let $\rho_n > 0$ be a sequence with $\rho_n \to 0$ as $n \to \infty$. We can assume that $u \in \mathcal{U}$ and $F_0(u) < +\infty$, since otherwise we had from Proposition 3.3.5 that $\liminf_{n\to\infty} F_{\rho_n}(u_n) = +\infty$ for any sequence $u_n \to u$ in $L^1(\Omega)$, and there were nothing to show.

We consider the sequence (u_n) in $\mathrm{GSBV}^2(\Omega)$ defined for all $n \in \mathbb{N}$ by

$$u_n(x_1,x_2,x_3) = u(x_1,x_2)\exp\Big(\frac{\lambda}{\lambda+2\mu}a^{\alpha\beta}b_{\alpha\beta}\rho_n x_3\Big) \quad \text{for all } x=(x_1,x_2,x_3)\in\Omega\,.$$

It is easy to see that $u_n \to u$ in $L^1(\Omega)$ as $n \to \infty$. We consider in the following again the identity (3.29) and show that each of the terms $I^{(k)}_{\rho_n}(u_n)$ (for $k = 1, 2, 3, 4$) converges in the right way.

Since all the functions in the exponential are uniformly bounded, there holds $|u_n| \le C|u|$ for some constant $C > 0$. Moreover, since b^σ_α is bounded, we deduce from (3.17)

$$\big|\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n)\big| = |\Lambda^3_{\alpha\beta,\rho_n}u_n| \le C|b_{\alpha\beta}u| + C\rho_n\sum_\sigma |b_{\sigma\beta}u|\,. \tag{3.33}$$

Because of our assumption, Remark 3.3.2 yields $(b_{\alpha\beta})u \in L^2(\Omega;\mathbb{R}^{2\times2})$, and thus the right hand side of (3.33) is also in $L^2(\Omega)$. From (3.21) (replacing λ by $\frac{2\lambda\mu}{\lambda+2\mu}$) we get that there exists $C > 0$ such that

$$\Big(\frac{2\lambda\mu}{\lambda+2\mu}g^{\alpha\beta}_{\rho_n}g^{\sigma\tau}_{\rho_n} + \mu(g^{\alpha\sigma}_{\rho_n}g^{\beta\tau}_{\rho_n} + g^{\alpha\tau}_{\rho_n}g^{\beta\sigma}_{\rho_n})\Big)\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n)\tilde{\boldsymbol{\epsilon}}_{\sigma\tau,\rho_n}(u_n) \le C\sum_{\alpha,\beta}\big|\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n)\big|^2$$

and therefore by the dominated convergence theorem

$$\lim_{n\to\infty} I^{(1)}_{\rho_n}(u_n) = \frac{1}{2}\int_\Omega \boldsymbol{c}^{\alpha\beta\sigma\tau}b_{\alpha\beta}b_{\sigma\tau}|u|^2\sqrt{a}\,\mathrm{d}x\,. \tag{3.34}$$

In the given setting we clearly have $\big|\tilde{\boldsymbol{\epsilon}}_{\alpha3}(u_n)\big| \le C|\partial_\alpha u| \in L^2(\Omega)$. In the same way as before, using (3.18), the dominated convergence theorem yields

$$\lim_{n\to\infty} I^{(3)}_{\rho_n}(u_n) = \frac{\mu}{2}\int_\Omega a^{\alpha\beta}\partial_\alpha u\partial_\beta u\sqrt{a}\,\mathrm{d}x\,. \tag{3.35}$$

We continue with the remark that

$$S_{u_n} = S_u\,,\quad (\nu_{u_n})_3 = 0 \quad\text{and}\quad [\nu_{u_n}]_\alpha = [\nu_u]_\alpha\,.$$

Hence, together with Proposition 3.2.4

$$I^{(4)}_{\rho_n} = \kappa\int_{S_u}\sqrt{[\nu_u]_\alpha g_{\rho_n}[\nu_u]_\beta}\sqrt{g_{\rho_n}}\,\mathrm{d}\mathcal{H}^2 \to \kappa\int_{S_u}\sqrt{[\nu_u]_\alpha a^{\alpha\beta}[\nu_u]_\beta}\sqrt{a}\,\mathrm{d}\mathcal{H}^2 \tag{3.36}$$

as $n \to \infty$.

It remains to show that $I^{(2)}_{\rho_n}(u_n) \to 0$. For that purpose, we note that

$$\tilde{\boldsymbol{\epsilon}}_{33,\rho_n}(u_n) = \frac{\lambda}{\lambda+2\mu}a^{\alpha\beta}b_{\alpha\beta}u_n$$

and therefore

$$\begin{aligned}|g^{\alpha\beta}_{\rho_n}\tilde{\boldsymbol{\epsilon}}_{\alpha\beta,\rho_n}(u_n)+a^{\alpha\beta}b_{\alpha\beta}u_n| &\leq |a^{\alpha\beta}-g^{\alpha\beta}_{\rho_n}||b_{\alpha\beta}u_n|+\rho_n|x_3 g^{\alpha\beta}_{\rho_n}b^{\sigma}_{\alpha}b_{\sigma\beta}u_n| \\ &\leq C\rho_n\sum_{\alpha,\beta}|b_{\alpha\beta}u|\,.\end{aligned}$$

Using once more that $b_{\alpha\beta}u\in L^2(\Omega)$ and the uniform bound of $\sqrt{g_{\rho_n}}$ we deduce

$$|I^{(2)}_{\rho_n}(u_n)|\leq\frac{C\rho_n^2}{2}\sum_{\alpha,\beta}\int_\Omega(\lambda+2\mu)|b_{\alpha\beta}u|^2\,\mathrm{d}x$$

such that $I^{(2)}_{\rho_n}(u_n)\to 0$. Eventually, together with (3.34), (3.35) and (3.36) we get $\lim_{n\to\infty}\mathcal{F}_{\rho_n}(u_n)=\mathcal{F}(u)$, which concludes the proof. □

Theorem 3.3.3 now follows directly from Proposition 3.3.5 and Proposition 3.3.6.

4 Phase Field Approximation of generalized Mumford-Shah Functionals

For numerical computation of minimizers some variational approximations in terms of Γ-convergence (see Section 2.3) turned out to be very useful. In this chapter we will discuss some generalizations of the phase field approximation of L. Ambrosio and V. M. Tortorelli in [12]. We consider the Mumford-Shah functional given by

$$\mathcal{MS}(u) := \frac{\alpha}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \gamma \mathcal{H}^1(S_u) \quad \text{for all } u \in \mathrm{GSBV}(\Omega)\,.$$

The idea of introducing a phase field variable which describes the discontinuity set of u goes back to [13]. In [12] they introduced the functionals

$$\mathcal{AT}_\varepsilon(u,v) = \int_\Omega (v^2+\eta_\varepsilon)|\nabla u|^2 \,\mathrm{d}x + \int_\Omega \frac{1}{4\varepsilon}(1-v)^2 + \varepsilon|\nabla v|^2 \,\mathrm{d}x \tag{4.1}$$

for $u \in H^1(\Omega)$ and $v \in H^1(\Omega;[0,1])$ and showed via a Γ-convergence argument that any limit point $(u,1)$ of a sequence of minimizers $(u_\varepsilon, v_\varepsilon)$ of $\mathcal{AT}_\varepsilon$ is a minimizer of $\mathcal{MS}$, provided that $\frac{\eta_\varepsilon}{\varepsilon} \to 0$. Many other approximations using a phase field variable for describing the discontinuity set of u has been been proven. Allowing higher order derivatives of the phase field has been studied e.g. in [25] and [37]. The Γ-convergence of $\mathcal{AT}_\varepsilon$ for other convergence behaviours of $\frac{\eta_\varepsilon}{\varepsilon}$ and other scalings of the different integral has been investigated in [56] and [82]. A totally different idea of approximating $\mathcal{MS}$ by finite differences was proposed by E. De Giorgi and proven by M. Gobbino in [76]. In [32] A. Braides and G. Dal Maso used non-local functionals depending on the average of the gradient of u on small balls. From the work presented in [34] one gets an approximation of $\mathcal{MS}$ for the following functional with small $\varepsilon > 0$:

$$\int_\Omega (v^2+\eta_\varepsilon)|\nabla u|^2 \,\mathrm{d}x + \frac{1}{2^{p'}\varepsilon}\int_\Omega (1-v)^{p'} \,\mathrm{d}x + \varepsilon^{p-1}\int_\Omega |\nabla v|^p \,\mathrm{d}x \tag{4.2}$$

for $u \in H^1(\Omega)$ and $v \in W^{1,p}(\Omega)$ with $p > 1$ and p' being the Hölder conjugate of p.

In all the approximations v works as a phase field variable describing the discontinuity set of u. To be more precise, for small $\varepsilon > 0$ the function v is close to 0 where u is "steep" or jumps, which means in the context of fracture mechanics the presence of a crack and in the context of image segmentation the presence of a segmentation contour. Elsewhere, the phase field variable is close to 1 and u is expected to be "flat" in this area. In practice the weights of the different integral terms declare what is meant to be "steep" or "flat".

In this chapter we show two novelties. In Section 4.1 we show a generalization of the Ambrosio-Tortorelli approximation. In (4.2) we replace the Euclidean norms of the gradients by any other norm, which may depend on the spatial variable x (see Theorem 4.1.2) and we allow the toughness also depend on x. As a special case we obtain in Section 4.2 a phase field approximation for the two-dimensional energy functional for thin elastic shells, which we derived in the previous chapter. Our result includes, moreover, the generalization that has been conjectured in [40], but has – as far as we know – not been proven, yet. This section is planned to be published in [3] with Stefano Almi as a coauthor.

In Section 4.3 we present a new approximation of the Mumford-Shah functional, allowing the phase field variable v to be in $\mathrm{BV}(\Omega)$, the set of functions of bounded variation. Precisely, in Corollary 4.3.3 we consider the functionals

$$\frac{\alpha}{2}\int_{\Omega}(v^2+\eta_\varepsilon)|\nabla u|^2\,\mathrm{d}x+\frac{\gamma}{2\varepsilon}\int_{\Omega}(1-v)\,\mathrm{d}x+\frac{\gamma}{2}|\mathrm{D}v|(\Omega)$$

for $u \in H^1(\Omega)$ and $v \in \mathrm{BV}(\Omega)$, which Γ-converge in some sense to $\mathcal{MS}$ and represents the case with $p = 1$ in (4.2).

In this way the phase field variable v can have jumps, which is exploited in the proof of Proposition 4.1.5, where we construct the recovery sequence for our Γ-convergence result. Moreover, we expect from this fact that the phase fields become sharper than the ones obtained from (4.1). In Section 4.4 we approve this expectation with some numerical computations in the context of segmental image denoising. The algorithm we use is also a new approach in this context. Instead of an alternating minimization, which has been frequently used e.g. in [27, 30] (see also Chapter 6), we use a new approach in this context. After the finite difference discretization we use a proximal alternating linearized minimization (PALM), which helps us to avoid solving linear systems. In this way we get a faster algorithm than from the pure alternating minimization.

These last two sections are the content of the paper [23] which arose from a collaboration with Kristian Bredies and which was submitted in March 2019. They are somewhat apart from the rest of this thesis, as we make no further use of the theoretical result and do not study the connection and the applicability to fracture. Indeed, there should be no problem in applying the same numerical technique to fracture in order to obtain analog results. However, in such simulations, it is quite common – not to say necessary – for efficiency reasons to use some adaptive mesh refinement as discussed in Chapter 6 (see also [16, 38]), which works only for finite element discretizations. On a finite difference grid one can only refine the mesh globally so that the advantage of mesh adaptation is lost. An extensive investigation of how to apply finite element methods to total variation minimization together with the right mesh adaption methods has yet not been realised.

4.1 Sobolev Phase Fields

We state here a generalization of the classical Ambrosio-Tortorelli approximation, which is applicable to the two-dimensionel shell model we derived in Chapter 3. The proof is based on the ideas from [34, Theorem 3.10], which states a related result for the perimeter functional. For a better readability we first summarize all the necessary assumptions.

Assumption 4.1.1. Let $\Omega \subset \mathbb{R}^n$ be a non-empty, open, bounded set with Lipschitz boundary, and assume that

(a) $f\colon [0,1] \to [0,\infty)$ is continuous and increasing with $f(0) = 0$,

(b) $W\colon [0,1] \to [0,\infty)$ is continuous and decreasing with $W(s) = 0$ if and only if $s = 1$,

(c) $\varphi_1, \varphi_2\colon \mathbb{R}^n \times \Omega \to \mathbb{R}$ are such that
   (i) $\varphi_1(\cdot, x)$ and $\varphi_2(\cdot, x)$ are norms in $\mathbb{R}^n$ for all $x \in \Omega$,
   (ii) there exists $C, c > 0$ with

$$c|\nu| \le \varphi_2(\nu, x) \le C|\nu| \quad \text{for all } x, \nu \in \mathbb{R}^n$$

   (iii) $\varphi_2(\nu, \cdot)$ is uniformly Lipschitz for every $\nu \in \mathbb{S}^{n-1}$, i.e. there exists an $L > 0$ such that

$$|\varphi_2(\nu, x) - \varphi_2(\nu, y)| \le L|x - y| \quad \text{for all } x, y \in \mathbb{R}^n, \nu \in \mathbb{S}^{n-1},$$

(d) $K\colon \Omega \to \mathbb{R}$ Lipschitz continuous with $\inf_\Omega K > 0$,

(e) $\eta_\varepsilon > 0$ for each $\varepsilon > 0$ such that $\frac{\eta_\varepsilon}{\varepsilon} \to 0$ as $\varepsilon \to 0$.

Now, we are ready to state the main theorem of this section.

Theorem 4.1.2. *Let $\Omega, f, W, \varphi_1, \varphi_2, K, \eta_\varepsilon$, be as in Assumption 4.1.1.*
For each $\varepsilon > 0$ we define the functionals $\mathcal{F}_\varepsilon\colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by

$$\mathcal{F}_\varepsilon(u, v) := \int_\Omega (f(v) + \eta_\varepsilon)\varphi_1^2(\nabla u, x)\,\mathrm{d}x + \int_\Omega \frac{1}{\varepsilon} W^2(v) K + \varepsilon \varphi_2^2(\nabla v, x)\,\mathrm{d}x \tag{4.3}$$

for all $u \in H^1(\Omega), v \in H^1(\Omega; [0,1])$ and $\mathcal{F}_\varepsilon(u, v) := +\infty$ otherwise.
Moreover, we define $\mathcal{F}\colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by

$$\mathcal{F}(u, v) := \int_\Omega f(1)\varphi_1^2(\nabla u, x)\,\mathrm{d}x + 4c_W \int_{S_u} \varphi_2(\nu_u, x)\sqrt{K}\mathcal{H}^{n-1}(x)$$

for $u \in \mathrm{GSBV}^2(\Omega)$ and $v = 1$ a.e., and $\mathcal{F}(u, v) = \infty$ otherwise, with $c_W := \int_0^1 W(s)\,\mathrm{d}s$.
Then there holds $F = \Gamma\text{-}\lim_{\varepsilon \to 0} \mathcal{F}_\varepsilon$.

The proof follows directly from Proposition 4.1.4 and Proposition 4.1.5 showing the Γ-lim inf-inequality and the Γ-lim sup-inequality, respectively.

First of all we show an auxiliary Γ-lim inf-inequality in one dimension.

Proposition 4.1.3. *Let $\Omega \subset \mathbb{R}, f, K, W, \eta_\varepsilon$ fulfill Assumption 4.1.1 and let $g, h \in C(\Omega)$ with strictly positive lower bound. We define for each $\varepsilon > 0$ the functional $\mathcal{F}_\varepsilon \colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by*

$$\mathcal{F}_\varepsilon(u,v) := \int_\Omega (f(v) + \eta_\varepsilon)|\nabla u|^2 g \,\mathrm{d}x + \int_\Omega \frac{1}{\varepsilon} W^2(v) K + \varepsilon |\nabla v|^2 h \,\mathrm{d}x$$

for all $u \in H^1(\Omega), v \in H^1(\Omega;[0,1])$ and $\mathcal{F}_\varepsilon(u,v) := +\infty$ otherwise. Furthermore, define $\mathcal{F} \colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by

$$\mathcal{F}(u,v) := \int_\Omega f(1)|\nabla u|^2 g \,\mathrm{d}x + 4c_W \sum_{x \in S_u} \sqrt{K(x)h(x)}$$

for $u \in \mathrm{SBV}^2(\Omega)$ and $v = 1$ a.e., and $\mathcal{F}(u,v) = +\infty$ otherwise, with $c_W := \int_0^1 W(s)\,\mathrm{d}s$.
Then there holds $F \leq \Gamma\text{-}\liminf_{\varepsilon \to 0} \mathcal{F}_\varepsilon$.

Proof. First of all we define for each open set $I \subset \Omega$ and $\varepsilon > 0$ the localized functionals

$$\mathcal{F}_\varepsilon(u,v;I) := \int_I (f(v) + \eta_\varepsilon)|u'|^2 g + \frac{1}{\varepsilon} W^2(v) K + \varepsilon |v'|^2 h \,\mathrm{d}x\,.$$

for $u \in H^1(\Omega)$, $v \in H^1(\Omega;[0,1])$ and $\mathcal{F}_\varepsilon(u,v;I) = +\infty$ otherwise.

Now, let $\varepsilon_j \to 0$ as $j \to \infty$, and let (u_j) and (v_j) be sequences in $L^1(\Omega)$ such that $u_j \to u$ and $v_j \to v$ as $j \to \infty$. We can assume (up to subsequence) that

$$\liminf_{j\to\infty} \mathcal{F}_{\varepsilon_j}(u_j, v_j) = \lim_{j\to\infty} \mathcal{F}_{\varepsilon_j}(u_j, v_j) < \infty \tag{4.4}$$

and, therefore, that $v = 1$ a.e.. Otherwise we would have $\frac{1}{\varepsilon}\int_\Omega W^2(v) K \,\mathrm{d}x \to \infty$ as $\varepsilon \to 0$, because of Assumption 4.1.1 (b).

The proof is divided in two main steps: For all $\delta > 0$ sufficiently small we firstly show that $\#S_u$ is finite and

$$4c_W \sum_{x \in S_u} \inf_{B_\delta(x)} \sqrt{Kh} \leq \liminf_{j\to\infty} \mathcal{F}_{\varepsilon_j}(u_j, v_j; B_\delta(S_u))\,, \tag{4.5}$$

and secondly we prove that

$$\int_{\Omega \setminus B_\delta(S_u)} f(1)|u'|^2 g \,\mathrm{d}x \leq \liminf_{j\to\infty} \mathcal{F}_{\varepsilon_j}(u_j, v_j; \Omega \setminus \overline{B_\delta(S_u)})\,. \tag{4.6}$$

In order to show (4.5), we take $y_0 \in S_u$, and let $\delta > 0$ sufficiently small such that $B_\delta(y_0) \subset \Omega$. Set $M := \liminf_{j\to\infty} \inf_{x \in B_{\frac{\delta}{2}}(y_0)} (f \circ v_j)$ and assume that $M > 0$. Note, that because of the Sobolev embeddings, we can assume that v_j is continuous, and therefore pointwise evaluations make sense. We take an arbitrary $0 < \rho < M$. Then, there exists $j_0 > 0$ such that up to subsequence there holds $M < \inf_{x \in B_{\frac{\delta}{2}}(y_0)} f(v_j(x)) + \rho$ for all $j > j_0$, and we can deduce

$$\int_{y_0 - \frac{\delta}{2}}^{y_0 + \frac{\delta}{2}} |u_j'|^2 \,\mathrm{d}x \leq \frac{C}{M - \rho} \int_{y_0 - \frac{\delta}{2}}^{y_0 + \frac{\delta}{2}} f(v_j)|u_j'|^2 g \,\mathrm{d}x \leq \frac{C}{M - \rho} \quad \text{for all } j > j_0$$

so that u_j converges weakly to u in $H^1(B_{\frac{\delta}{2}}(y_0))$ and consequently we get the contradiction $y_0 \notin S_u$. Hence, we must have $M = 0$. Because of the assumptions on f (see Assumption 4.1.1 (a)) we can find a sequence (y_j) in $B_{\frac{\delta}{2}}(y_0)$ such that $v_j(y_j) \to 0$. Since $v_j \to 1$ a.e. there exist $y^+, y^- \in B_\delta(y_0)$ such that $y^- < y_0 < y^+$ and $v_j(y^-) \to 1$ as well as $v_j(y^+) \to 1$.

With this at hand we have

$$2c_W = \lim_{j\to\infty} \left[\int_{v_j(y_j)}^{v_j(y^+)} W(s)\,\mathrm{d}s + \int_{v_j(y_j)}^{v_j(y^-)} W(s)\,\mathrm{d}s \right]. \tag{4.7}$$

Defining

$$\Phi_j(t) := \int_0^{v_j(t)} W(s)\,\mathrm{d}s \qquad \text{and} \qquad \gamma := \inf_{B_\delta(y_0)} \sqrt{Kh}$$

we can estimate

$$\begin{aligned} \gamma \int_{v_j(y_j)}^{v_j(y^+)} W(s)\,\mathrm{d}s + \gamma \int_{v_j(y_j)}^{v_j(y^-)} W(s)\,\mathrm{d}s &= \gamma \int_{y_j}^{y^+} \Phi_j'(t)\,\mathrm{d}t + \gamma \int_{y_j}^{y^-} \Phi_j'(t)\,\mathrm{d}t \\ &\le \gamma \int_{y_0-\delta}^{y_0+\delta} |\Phi_j'(t)|\,\mathrm{d}t \\ &\le \int_{y_0-\delta}^{y_0+\delta} W(v_j)\sqrt{K}\,|v_j'|\sqrt{h}\,\mathrm{d}x\,. \end{aligned} \tag{4.8}$$

Continuing with Young's inequality we obtain

$$\begin{aligned} 2\int_{y_0-\delta}^{y_0+\delta} W(v_j)\sqrt{K}\,|v_j'|\sqrt{h}\,\mathrm{d}x &\le \int_{y_0-\delta}^{y_0+\delta} \frac{1}{\varepsilon} W^2(v_j)K + \varepsilon |v_j'|^2 h\,\mathrm{d}x \\ &\le \mathcal{F}_{\varepsilon_j}(u_j, v_j; B_\delta(y_0))\,. \end{aligned} \tag{4.9}$$

Thus, together with (4.7) and (4.8) we have for all $\delta > 0$ sufficiently small

$$4c_W \inf_{B_\delta(y_0)} \sqrt{Kh} \le \liminf_{j\to 0} \mathcal{F}_{\varepsilon_j}(u_j, v_j; B_\delta(y_0))\,.$$

For each element in any discrete set $\{y_1, \dots, y_N\} \subset S_u$ (with $N < \#S_u$) we can repeat the preceding arguments in order to obtain

$$4c_W \sum_{i=1}^N \inf_{B_\delta(y_i)} \sqrt{Kh} \le \liminf_{j\to 0} \mathcal{F}_{\varepsilon_j}\Big(u_j, v_j; \bigcup_{i=1}^N B_\delta(y_i)\Big)$$

for all $\delta > 0$ so small that $B_\delta(y_k) \cap B_\delta(y_\ell) = \emptyset$ for $k \neq \ell$. Because of (4.4) the right hand side is finite, and we therefore must have that $\#S_u$ is finite, and we can conclude with (4.5).

For proving (4.6) let $I := (a, b) \subset \Omega$ be an open interval such that $I \cap S_u = \emptyset$. For $k \in \mathbb{N}$ and $\ell \in \{1, \dots, n\}$ we define the intervals

$$I_\ell^k := \Big(a + \frac{\ell - 1}{k}(b - a), a + \frac{\ell}{k}(b - a)\Big)$$

and we extract a subsequence of v_j (not relabeled) such that $\lim_{j\to\infty}\inf_{x\in I^k_\ell} v_j(x)$ exists for all k. Moreover, for $0<z<1$ we define the set

$$T^k_z := \Big\{\ell \in \{1,\dots,k\}\colon \lim_{j\to\infty}\inf_{x\in I^k_\ell} v_j(x) \le z\Big\}\,.$$

For any $\ell \in T^k_z$ there exists a sequence (x_j) in I^k_ℓ and $y \in I^k_\ell$ such that

$$\lim_{j\to\infty} v_j(x_j) = \lim_{j\to\infty}\inf_{x\in I^k_\ell} v_j(x) \quad \text{and} \quad v_j(y)\to 1\,.$$

With this at hand we can estimate precisely as in (4.8) and (4.9), using Assumption 4.1.1 (d) and $\inf_\Omega g > 0$,

$$\int_z^1 W(s)\,\mathrm{d}s \le \lim_{j\to\infty}\int_{v_j(x_j)}^{v_j(y)} W(s)\,\mathrm{d}s \le C\liminf_{j\to\infty}\mathcal{F}_{\varepsilon_j}(u_j,v_j;I^k_\ell)\,.$$

where the right hand side is uniformly bounded by assumption.

Repeating this argument for every $\ell\in T^k_z$ we get

$$\#(T^k_z) \le C\Big(\int_z^1 W(s)\,\mathrm{d}s\Big)^{-1}\,.$$

Now, for every k large enough we can select $\ell^k_1 < \ell^k_2 < \cdots < \ell^k_N \in T^k_z$ with $N = \max_{k\in\mathbb{N}}\#(T^k_z)$ independent of k, such that $\frac{\ell^k_i}{k}$ converges to some $y_i\in\bar I$ as $k\to\infty$ for all $i\in\{1,\dots,N\}$. Define $T_z=\{y_1,\dots,y_N\}$; let $\delta>0$, and choose $k>\frac{b-a}{2\delta}$ and $\ell\in T^k_z$. Then we have $I^k_\ell\subset B_\delta(T_z)$. Therefore,

$$\begin{aligned}\liminf_{j\to\infty} f(z)\int_{I\setminus B_\delta(T_z)} |u_j'|^2 g\,\mathrm{d}x &\le \liminf_{j\to\infty}\int_I f(v_j)|u_j'|^2 g\,\mathrm{d}x\\ &\le \liminf_{j\to\infty}\mathcal{F}_{\varepsilon_j}(u_j,v_j;I)\end{aligned}$$

Since $\delta>0$ was chosen arbitrarily it is possible to integrate over $I\setminus T_z$ on the left hand side. From there, we obtain $u_j'\rightharpoonup u'$ in $L^2(I\setminus T_z)$ as $j\to\infty$ up to subsequences. By Sobolev embedding we get $u\in H^1(I\setminus T_z)$, and since $S_u\cap I=\emptyset$ there even holds $u\in H^1(I)$. Using the weakly lower semi-continuity of the norm and letting $z\to 1$ we get

$$\int_I f(1)|u'|^2\,\mathrm{d}x \le \liminf_{j\to\infty}\mathcal{F}_{\varepsilon_j}(u_j,v_j;I)\,.$$

Since $I\subset\Omega$ was chosen arbitrarily such that $I\cap S_u=\emptyset$ we conclude with (4.6).

Summing (4.5) and (4.6) we get

$$\int_{\Omega\setminus B_\delta(S_u)} f(1)|u'|^2 g\,\mathrm{d}x + 4c_W\sum_{x\in S_u}\inf_{B_\delta(x)}\sqrt{Kh} \le \liminf_{j\to\infty}\mathcal{F}_{\varepsilon_j}(u_j,v_j;\Omega)\,.$$

Using the continuity of K (see Assumption 4.1.1 (d)) and h, for $\delta\to 0$ we eventually get $\mathcal{F}(u,v)\le\liminf_{j\to\infty}\mathcal{F}_{\varepsilon_j}(u_j,v_j)$.

□

The generalization of the Γ-lim inf-inequality to any dimension $n \in \mathbb{N}$ now follows by a slicing argument. It is based on Theorem 2.4.2. We also use the notation described in that context.

Proposition 4.1.4. *In the setting of Theorem 4.1.2 there holds*

$$\mathcal{F}(u,v) \le \Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon(u,v) \quad \textit{for all } u,v \in L^1(\Omega)\,.$$

Proof. In what follows we use the notation for slicing introduced in Section 2.4. Let $A \subset \Omega$ be open, $\xi \in \mathbb{S}^{n-1}$ and $y \in A_\xi$.

We define the localized version of (4.3) by

$$\mathcal{F}_\varepsilon(u,v;A) := \int_A f(v)\varphi_1^2(\nabla u, x)\,\mathrm{d}x + \int_A \frac{1}{\varepsilon}W^2(v)K + \varepsilon\varphi_2^2(\nabla v, x)\,\mathrm{d}x$$

if $u \in H^1(A), v \in H^1(A;[0,1])$ and $\mathcal{F}_\varepsilon(u,v;A) := +\infty$ otherwise. Furthermore, we denote by $\varphi_1^*(\cdot,x)$ and $\varphi_2^*(\cdot,x)$ the dual norm of $\varphi_1(\cdot,x)$ and $\varphi_2(\cdot,x)$, respectively, for all $x \in \Omega$. Note that there holds

$$\varphi_i(\zeta,x) = \sup_{\substack{z\in\mathbb{R}^n \\ \varphi_i^*(z,x)\le 1}} \big|\langle\zeta,z\rangle\big| = \sup_{z\in\mathbb{S}^{n-1}} \frac{\big|\langle\zeta,z\rangle\big|}{\varphi_i^*(z,x)} \quad \text{for all } \zeta\in\mathbb{R}^n, x\in\Omega\,. \tag{4.10}$$

For $I \subset \mathbb{R}$ we define

$$\mathcal{F}_\varepsilon^{\xi,y}(u,v;I) := \int_I f(v)\frac{|u'|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x + \frac{1}{\varepsilon}\int_I W^2(v)K\,\mathrm{d}x + \varepsilon\int_I \frac{|v'|^2}{(\varphi_2^*)^2(\xi,x)}\,\mathrm{d}x$$

if $u \in H^1(I), v\in H^1(I;[0,1])$ and $\mathcal{F}_\varepsilon^{\xi,y}(u,v;I) := +\infty$ otherwise. Now, we set for all $u,v \in L^1(\Omega)$

$$\mathcal{F}_\varepsilon^{\xi}(u,v;A) := \int_{A_\xi} \mathcal{F}_\varepsilon^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi)\mathrm{d}\mathcal{H}^{n-1}(y)\,.$$

Thus, we have by Fubini's theorem

$$\mathcal{F}_\varepsilon^{\xi}(u,v;A) = \int_A f(v)\frac{\big|\langle\nabla u,\xi\rangle\big|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x + \frac{1}{\varepsilon}\int_A W^2(v)K\,\mathrm{d}x + \varepsilon\int_A \frac{\big|\langle\nabla v,\xi\rangle\big|}{(\varphi_2^*)^2(\xi,x)}\,\mathrm{d}x$$

if $|\langle \mathrm{D}u,\xi\rangle|(A)$ is absolutely continuous with respect to $\mathcal{L}^n$ and if $|\langle Dv,\xi\rangle|(A) < \infty$, and $\mathcal{F}_\varepsilon^\xi(u,v;A) = +\infty$ otherwise, and there clearly holds

$$\mathcal{F}_\varepsilon^\xi(u,v;A) \le \mathcal{F}_\varepsilon(u,v;A)\,. \tag{4.11}$$

From Proposition 4.1.3 we know that $\mathcal{F}^{\xi,y}(u,v;I) \le \Gamma\text{-}\liminf_{\varepsilon\to 0}\mathcal{F}_\varepsilon^{\xi,y}(u,v;I)$ with

$$\mathcal{F}^{\xi,y}(u,v;I) := \int_I f(1)\frac{|u'|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x + 4c_W\sum_{x\in S_u}\frac{\sqrt{K(x)}}{\varphi_2^*(\xi,x)}$$

for $u \in \mathrm{SBV}^2(I), v = 1$ a.e. and $\mathcal{F}^{\xi,y}(u,v;I) := +\infty$ otherwise. We now define

$$\mathcal{F}^{\xi}(u,v;A) := \int_{A_\xi} \mathcal{F}^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi)\,\mathrm{d}\mathcal{H}^{n-1}(y)\,,$$

and show that

$$\mathcal{F}^{\xi}(u,v;A) \le \Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon^{\xi}(u,v;A) \le \Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{F}_\varepsilon(u,v;A)\,. \tag{4.12}$$

Let (u_ε) and (v_ε) with $u_\varepsilon \to u$ and $v_\varepsilon \to v$ in $L^1(\Omega)$ as $\varepsilon \to 0$. We extract a subsequence ε_j such that

$$\liminf_{\varepsilon\to 0} F_\varepsilon^{\xi}(u_\varepsilon, v_\varepsilon; A) = \lim_{j\to\infty} F_{\varepsilon_j}^{\xi}(u_{\varepsilon_j}, v_{\varepsilon_j}; A)\,. \tag{4.13}$$

By Fubini's Theorem we get that

$$\|u_{\varepsilon_j} - u\|_{L^1(A)} = \int_{A_\xi}\int_{A_y^\xi} |(u_{\varepsilon_j})_y^\xi(t) - u_y^\xi(t)|\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}(y) \to 0 \quad \text{as } j\to\infty\,.$$

From this we infer that for $\xi \in \mathbb{S}^{n-1}$ and for almost all $y \in A_\xi$ there exists a subsequence u_{ε_j} (not relabled) such that $(u_{\varepsilon_j})_y^\xi \to u_y^\xi$ as $j\to\infty$ in $L^1(A_y^\xi)$. Consequently, from Proposition 4.1.3 we obtain

$$\mathcal{F}^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi) \le \liminf_{j\to\infty} \mathcal{F}_{\varepsilon_j}^{\xi,y}((u_{\varepsilon_j})_y^\xi, (v_{\varepsilon_j})_y^\xi, A_y^\xi)\,.$$

From Fatou's Lemma, from (4.13) and from (4.11) we deduce

$$\mathcal{F}^{\xi}(u,v;A) \le \liminf_{j\to\infty} F_{\varepsilon_j}^{\xi}(u_{\varepsilon_j}, v_{\varepsilon_j}; A) = \liminf_{\varepsilon\to 0} F_\varepsilon^{\xi}(u_\varepsilon, v_\varepsilon; A) \le \liminf_{\varepsilon\to 0} F_\varepsilon(u_\varepsilon, v_\varepsilon; A)$$

We conclude (4.12), since $(u_\varepsilon, v_\varepsilon)$ was chosen arbitrarily.

Next, we show that if F^ξ is finite there holds $u \in \mathrm{GSBV}^2(A)$ and $v = 1$ a.e. on A. We know that $\mathcal{F}^\xi(u,v;A)$ is finite if and only if for a.a. $y \in A_\xi$ there holds $v_y^\xi = 1$ a.e. on A_y^ξ, $u_y^\xi \in \mathrm{SBV}^2(A_y^\xi)$ and

$$\int_{A_\xi}\int_{A_y^\xi} f(1)\frac{|\nabla u_y^\xi|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x\,\mathrm{d}\mathcal{H}^{n-1}(y) + 4c_W \int_{A_\xi} \sum_{x\in S_{u_y^\xi}} \frac{\sqrt{K(x)}}{\varphi_2^*(\xi,x)}\,\mathrm{d}\mathcal{H}^{n-1}(y) < \infty\,.$$

Since there holds for every $M > 0$ and every $u \in L^1(\Omega)$ with $u_y^\xi \in \mathrm{SBV}^2(A_y^\xi)$ for a.a. $y \in A_\xi$

$$\begin{aligned} &\int_{A_\xi} \big|\mathrm{D}(-M \vee u_y^\xi \wedge M)\big|(A_y^\xi)\mathrm{d}\mathcal{L}^{n-1}(y) \\ \le &\int_{A_\xi} \frac{1}{4}\mathcal{L}^1(A_y^\xi) + \|(-M \vee u_y^\xi \wedge M)'\|^2_{L^2(A_y^\xi)} + 2M\#S_{u_y^\xi}\,\mathrm{d}\mathcal{H}^{n-1}(y) \end{aligned}$$

$$\leq \frac{1}{4}\mathcal{L}^n(A) + C\int_{A_y^\xi} F^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi)\,\mathrm{d}\mathcal{H}^{n-1}(y)$$

we get by Corollary 2.4.3 that $\mathcal{F}^\xi(u,v;A)$ is finite only if $u \in \mathrm{GSBV}^2(A)$ and $v = 1$ a.e. in A. Hence,

$$\mathcal{F}^\xi(u,v;A) = \int_A f(1)\frac{|\langle \nabla u, \xi\rangle|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x + \int_{S_u}\frac{|\langle \nu_u, \xi\rangle|}{\varphi_2^*(\xi,x)}\sqrt{K}\,\mathrm{d}\mathcal{H}^{n-1}$$

if $u \in \mathrm{GSBV}^2(A)$ and $\mathcal{F}^\xi(u,v;A) = \infty$ otherwise. Since A and ξ where chosen arbitrarily, a localization argument (see e.g. [34, Theorem 1.16]), (4.12) and (4.10) imply

$$\begin{aligned}\mathcal{F}(u,v;A) &= \int_A f(1)\varphi_1^2(\nabla u, x)\,\mathrm{d}x + \int_{S_u}\varphi_2(\nu_u,x)\sqrt{K}\,\mathrm{d}\mathcal{H}^{n-1}\\ &= \int_A f(1)\sup_{\xi\in\mathbb{S}^{n-1}}\frac{|\langle \nabla u, \xi\rangle|^2}{(\varphi_1^*)^2(\xi,x)}\,\mathrm{d}x + 2c_W\int_{S_u}\sup_{\xi\in\mathbb{S}^{n-1}}\frac{|\langle \nu_u, \xi\rangle|}{\varphi_2^*(\xi,x)}\sqrt{K}\,\mathrm{d}\mathcal{H}^{n-1}\\ &\leq \Gamma\text{-}\liminf_{\varepsilon\to 0}\mathcal{F}_\varepsilon(u,v;A)\end{aligned}$$

for $u \in \mathrm{GSBV}^2(A)$ and $v = 1$ a.e. on A. Otherwise, the lim inf-inequality follows directly from (4.12) with ξ being arbitrary. ☐

We are now ready to show the lim sup-inequality, which concludes the proof of Theorem 4.1.2.

Proposition 4.1.5. *In the setting of Theorem 4.1.2 there holds*

$$\Gamma\text{-}\limsup_{\varepsilon\to 0}\mathcal{F}_\varepsilon(u,v) \leq \mathcal{F}(u,v) \quad \textit{for all } u,v \in L^1(\Omega)$$

Proof. Throughout the proof $C > 0$ denotes an arbitrary constant greater than zero, which may vary from line to line in the computations below.

We clearly can assume that $\mathcal{F}(u,v) < +\infty$, and hence that $u \in \mathrm{GSBV}^2(\Omega)$ and $v = 1$ a.e. on Ω. We first show the inequality for $u \in \mathrm{SBV}^2(\Omega)$, such that

(a) $\overline{S_u}$ is the intersection of Ω with a finite number of pairwise disjoint $n-1$-simplexes,

(b) $\mathcal{H}^{n-1}(\overline{S_u}\setminus S_u) = 0$,

(c) $u \in W^{k,\infty}(\Omega\setminus\overline{S_u})$ for all $k \in \mathbb{N}$.

By the density result from Theorem 2.4.1 we then infer the lim sup-inequality for all $u \in \mathrm{SBV}^2(\Omega)\cap L^\infty(\Omega)$ and finally by a standard truncation argument we obtain the result for every $u \in \mathrm{GSBV}^2(\Omega)$.

For now let $u \in \mathrm{SBV}^2(\Omega)$ satisfying (a)–(c) above. For the construction of a recovery sequence of u we choose a smooth cut off function $\phi\colon \mathbb{R}\to\mathbb{R}$ with $\phi = 1$ on $B_{\frac{1}{2}}(0)$ and $\phi = 0$ on $\mathbb{R}\setminus B_1(0)$. For all $x \in \Omega$ define $\tau(x) = \mathrm{dist}(x, S_u)$ and $\phi_\varepsilon(x) = \phi(\frac{\tau(x)}{\delta_\varepsilon})$ for all $\varepsilon > 0$, where $\delta_\varepsilon := \sqrt{\varepsilon\eta_\varepsilon}$. In this way we have $\frac{\delta_\varepsilon}{\varepsilon} \to 0$ and $\frac{\eta_\varepsilon}{\delta_\varepsilon} \to 0$ as $\varepsilon \to 0$. Now, consider the functions $u_\varepsilon = (1-\phi_\varepsilon)u$ on Ω for every $\varepsilon > 0$. We then have $u_\varepsilon \in H^1(\Omega)$, $u_\varepsilon = u$ on $\Omega \setminus B_{\delta_\varepsilon}(S_u)$ and $u_\varepsilon \to u$ in $L^1(\Omega)$.

In order to construct the corresponding recovery sequence for $v = 1$ a.e. we define $\sigma\colon [0,\infty) \to [0,1]$ by the initial value problem:

$$\sigma' = W(\sigma)\,, \qquad \sigma(0) = 0\,.$$

We note that σ is an increasing Lipschitz continuous function sucht that $\sigma(t) \to 1$ as $t \to \infty$. Furthermore, the image set $\sigma^{-1}(t)$ is single valued for $t < 1$, and we can consider $\sigma^{-1}\colon [0,1) \to [0,\infty)$ as a continuous function.

For the following we set

$$\tilde{\varphi}_2(\zeta, x) := \frac{\varphi_2(\zeta, x)}{\sqrt{K(x)}} \quad \text{and} \quad \tilde{\tau}(x) = \frac{\tau(x)}{\tilde{\varphi}_2(\nabla\tau(x), x)} \quad \text{for all } \zeta \in \mathbb{R}^n, x \in \Omega\,.$$

Note that from our assumption on φ_2 and K and from Lemma 2.1.1 we can define $0 < d := \inf_{x\in\Omega} \tilde{\varphi}_2(\nabla\tau(x), x)$ and $\infty > D := \sup_{x\in\Omega} \tilde{\varphi}_2(\nabla\tau(x), x)$. Furthermore, we choose $\tilde{\delta}_\varepsilon := \frac{\delta_\varepsilon}{\varepsilon d}$ for all $\varepsilon > 0$ and a positive sequence (γ_ε) such that $\gamma_\varepsilon \to 0$ and $\varepsilon\sigma^{-1}\big(\frac{1}{1+\gamma_\varepsilon}\big) \to 0$ as $\varepsilon \to 0$. With this at hand we have for

$$\rho_\varepsilon := D\varepsilon\left(\sigma^{-1}\left(\frac{1}{1+\gamma_\varepsilon}\right) + \tilde{\delta}_\varepsilon\right)$$

that $\rho_\varepsilon \to 0$ as $\varepsilon \to 0$. Now we define for all $t > 0$ and for all $x \in \Omega$

$$\sigma_\varepsilon(t) := \begin{cases} 0 & \text{for } t \in [0, \tilde{\delta}_\varepsilon) \\ \min\{1, (1+\gamma_\varepsilon)\sigma(t - \tilde{\delta}_\varepsilon)\} & \text{otherwise} \end{cases} \quad \text{and} \quad v_\varepsilon(x) := \sigma_\varepsilon\left(\frac{\tilde{\tau}(x)}{\varepsilon}\right).$$

It is easy to check, that the way we have chosen all the parameters yields $v_\varepsilon = 1$ on $\Omega \setminus B_{\rho_\varepsilon}(S_u)$ and $v_\varepsilon = 0$ on $B_{\delta_\varepsilon}(S_u)$ for sufficiently small $\varepsilon > 0$.

The sequence $(u_\varepsilon, v_\varepsilon)$ will now serve as the recovery sequence for (u, v). We plug this into $\mathcal{F}_\varepsilon$ and obtain for sufficiently small $\varepsilon > 0$

$$\begin{aligned} \mathcal{F}_\varepsilon(u_\varepsilon, v_\varepsilon) = & \int_{\Omega\setminus B_{\delta_\varepsilon}(S_u)} f(v_\varepsilon)\varphi_1^2(\nabla u_\varepsilon, x)\,\mathrm{d}x + \eta_\varepsilon \int_\Omega \varphi_1^2(\nabla u_\varepsilon, x)\,\mathrm{d}x \\ & + \frac{1}{\varepsilon}\int_{B_{\delta_\varepsilon}(S_u)} W^2(0)K\,\mathrm{d}x \\ & + \int_{B_{\rho_\varepsilon}(S_u)\setminus B_{\delta_\varepsilon}(S_u)} \left(\frac{1}{\varepsilon}W^2(v_\varepsilon) + \varepsilon\tilde{\varphi}_2^2(\nabla v_\varepsilon, x)\right)K\,\mathrm{d}x, \end{aligned} \tag{4.14}$$

where we applied $f(0) = 0$ and $W(1) = 0$ from Assumption 4.1.1 (a) and (b), respectively, as well as the fact that $\nabla v_\varepsilon = 0$ on $B_{\delta_\varepsilon}(S_u)$ and on $\Omega \setminus B_{\rho_\varepsilon}(S_u)$. We continue using f being increasing from Assumption 4.1.1 (a) and obtain

$$\int_{\Omega\setminus B_{\delta_\varepsilon}(S_u)} f(v_\varepsilon)\varphi_1^2(\nabla u_\varepsilon, x)\,\mathrm{d}x \le \int_\Omega f(1)\varphi_1^2(\nabla u, x)\,\mathrm{d}x\,. \tag{4.15}$$

By construction of ϕ_ε and u_ε and with Lemma 2.1.1 we deduce $\|\nabla\phi_\varepsilon\|_{L^\infty(B_{\frac{\delta_\varepsilon}{2}}(S_u))} = 0$ and $\|\nabla\phi_\varepsilon\|_{L^\infty(\Omega)} \leq \frac{C}{\delta_\varepsilon}$. Taking into account that $\|u\|_{L^\infty(\Omega\setminus\overline{S_u})} \leq C$ we hence have on $B_{\delta_\varepsilon}(S_u)$

$$|\nabla u_\varepsilon| \leq |u\nabla\phi_\varepsilon| + \big|(1-\phi_\varepsilon)\nabla u\big| \leq \frac{C}{\delta_\varepsilon} + |\nabla u|\,.$$

This implies with Assumption 4.1.1 (c) (ii)

$$\eta_\varepsilon \int_\Omega \varphi_1^2(\nabla u_\varepsilon, x)\,\mathrm{d}x \leq C\eta_\varepsilon \int_\Omega |\nabla u_\varepsilon|^2\,\mathrm{d}x \leq C\eta_\varepsilon \int_\Omega |\nabla u|^2\,\mathrm{d}x + C\frac{\eta_\varepsilon}{\delta_\varepsilon^2}\mathcal{L}^n(B_{\delta_\varepsilon}(S_u))\,. \tag{4.16}$$

For compact subsets of a $(n-1)$-dimensional plane the Hausdorff measure coincides with the Minkowski content (see, e.g., [10, Section 2.13] or [62, Theorem 3.2.29]). Hence, by the structure of $\overline{S_u}$ there holds

$$\frac{\mathcal{L}^n(B_{\delta_\varepsilon}(\overline{S_u}))}{\delta_\varepsilon} \to 2\mathcal{H}^{n-1}(\overline{S_u}) \quad \text{as } \varepsilon \to 0\,, \tag{4.17}$$

and, since $\frac{\eta_\varepsilon}{\delta_\varepsilon} \to 0$ as $\varepsilon \to 0$ by the choice of δ_ε, (4.16) yields

$$\eta_\varepsilon \int_\Omega \varphi_1^2(\nabla u_\varepsilon, x)\,\mathrm{d}x \to 0 \quad \text{as } \varepsilon \to 0\,. \tag{4.18}$$

Since K is uniformly bounded on Ω (see Assumption 4.1.1 (d)), recalling $\frac{\delta_\varepsilon}{\varepsilon} \to 0$ as $\varepsilon \to 0$, we also infer from (4.17) that

$$\frac{1}{\varepsilon}\int_{B_{\delta_\varepsilon}(S_u)} W^2(0)K\,\mathrm{d}x \leq \frac{C}{\varepsilon}\mathcal{L}^n\big(B_{\delta_\varepsilon}(S_u)\big)W^2(0) \to 0 \quad \text{as } \varepsilon \to 0\,. \tag{4.19}$$

It remains to consider the limit behaviour of the last term of (4.14) which we abbreviate in the following way

$$\mathcal{G}_\varepsilon(v_\varepsilon) := \int_{B_{\rho_\varepsilon}(S_u)\setminus B_{\delta_\varepsilon}(S_u)} \Big(\frac{1}{\varepsilon}W^2(v_\varepsilon) + \varepsilon\tilde{\varphi}_2^2(\nabla v_\varepsilon, x)\Big)K\,\mathrm{d}x\,.$$

We need to show that

$$\limsup_{\varepsilon\to 0}\mathcal{G}_\varepsilon(v_\varepsilon) \leq 4c_W \int_{S_u} \varphi_2\big(\nu_u(x), x\big)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,. \tag{4.20}$$

Together with (4.15), (4.16), (4.18) and (4.19) plugged into (4.14) we would then obtain

$$\limsup_{\varepsilon\to 0}\mathcal{F}_\varepsilon(u_\varepsilon, v_\varepsilon) \leq \int_\Omega f(1)\varphi_1^2(\nabla u, x)\,\mathrm{d}x + 4c_W\int_{S_u}\varphi_2\big(\nu_u(x), x\big)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

Using the density result described in Theorem 2.4.1 and the lower semi-continuity of Γ-$\limsup \mathcal{F}_\varepsilon$ we get the assertion for any $u \in \mathrm{SBV}^2(\Omega)\cap L^\infty(\Omega)$. By a simple tuncation argument it follows for $u \in \mathrm{GSBV}^2(\Omega)$.

It remains to show (4.20). From the assumption on $\overline{S_u}$ we can write $\overline{S}_u = \bigcup_{i=1}^N \overline{S_u^i}$ for some $N \in \mathbb{N}$ and $\{\overline{S_u^1}, \dots, \overline{S_u^N}\}$ being a set of pairwise disjoint $(n-1)$-simplexes. With this at hand we can write for sufficiently small $\varepsilon > 0$

$$\mathcal{G}_\varepsilon(v_\varepsilon) = \sum_{i=1}^N \int_{B_{\rho_\varepsilon}(S_u^i) \setminus B_{\delta_\varepsilon}(S_u^i)} \Big(\frac{1}{\varepsilon} W^2(v_\varepsilon) + \varepsilon \tilde{\varphi}_2^2(\nabla v_\varepsilon, x) \Big) K \,\mathrm{d}x \,.$$

Hence, without loss of generality we assume in the following that $\overline{S_u}$ itself is a $(n-1)$-simplex. We consider the $(n-1)$-dimensional hyperplane, which contains S_u, say $\nu_u^\perp$ with ν_u being the unit normal of S_u.

We split the integration domain of $\mathcal{G}_\varepsilon$ in several parts. Precisely, we define

$$S_u^{-\perp} := \{x \in \Omega : x = y + t\nu_u \text{ for some } y \in S_u \text{ and } t < 0\}$$

and

$$S_u^{+\perp} := \{x \in \Omega : x = y + t\nu_u \text{ for some } y \in S_u \text{ and } t > 0\} \,,$$

and consider with $S_u^\perp := S_u^{-\perp} \cup S_u^{+\perp}$

$$\mathcal{G}_\varepsilon(v_\varepsilon) = \mathcal{G}_\varepsilon|_{S_u^{+\perp}} + \mathcal{G}_\varepsilon|_{S_u^{-\perp}} + \mathcal{G}_\varepsilon|_{\Omega \setminus S_u^\perp} \,,$$

where we define for every $A \subset \Omega$

$$G_\varepsilon|_A = \int_{A \cap B_{\rho_\varepsilon}(S_u) \setminus B_{\delta_\varepsilon}(S_u)} \Big(\frac{1}{\varepsilon} W^2(v_\varepsilon) + \varepsilon \tilde{\varphi}_2^2(\nabla v_\varepsilon, x) \Big) K \,\mathrm{d}x \,.$$

First of all note that we generally have for all $x \in \Omega \setminus \overline{S_u}$

$$\nabla v_\varepsilon(x) = \frac{1}{\varepsilon} \sigma_\varepsilon' \Big(\frac{\tilde{\tau}(x)}{\varepsilon} \Big) \Big(\frac{\nabla \tau(x)}{\tilde{\varphi}_2(\nabla \tau(x), x)} - \frac{\tau(x) \nabla \big[x \mapsto \tilde{\varphi}_2(\nabla \tau(x), x) \big]}{\tilde{\varphi}_2^2(\nabla \tau(x), x)} \Big) \,. \tag{4.21}$$

On $S_u^{+\perp}$ we have from Lemma 2.1.1 that $\nabla \tau(x) = \nu_u$ is constant and thus from Assumption 4.1.1 (c) and (d) we get that $x \mapsto \tilde{\varphi}_2(\nu_u, x)$ is Lipschitz. Hence, (4.21) yields

$$\tilde{\varphi}_2^2(\nabla v_\varepsilon(x), x) \le \frac{1}{\varepsilon^2} \Big| \sigma_\varepsilon' \Big(\frac{\tilde{\tau}(x)}{\varepsilon} \Big) \Big|^2 \big(1 + C\tau(x) \big)^2 \,,$$

and we can estimate

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1 + C\rho_\varepsilon)^2 \int_{S_u^{+\perp} \cap B_{\rho_\varepsilon}(S_u) \setminus B_{\delta_\varepsilon}(S_u)} \Bigg(\frac{1}{\varepsilon} (W^2 \circ \sigma_\varepsilon) \Big(\frac{\tilde{\tau}(x)}{\varepsilon} \Big) + \frac{1}{\varepsilon} \Big| \sigma_\varepsilon' \Big(\frac{\tilde{\tau}(x)}{\varepsilon} \Big) \Big|^2 \Bigg) K(x) \,\mathrm{d}x \,.$$

Together with the coarea formula (see e.g. [10, Theorem 2.93]) we obtain

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1+C\rho_\varepsilon)^2 \int_{\delta_\varepsilon}^{\rho_\varepsilon} \int_{S_u^{+\perp}\cap \partial B_t(S_u)} \bigg(\frac{1}{\varepsilon}(W^2\circ\sigma_\varepsilon)\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nu_u,x)}\Big) + \frac{1}{\varepsilon}\Big|\sigma_\varepsilon'\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nu_u,x)}\Big)\Big|^2\bigg) K(x)\,\mathrm{d}\mathcal{H}^{n-1}(x)\,\mathrm{d}t\,.$$

We apply the coordinate transformation $x \mapsto x + t\nu_u$ which maps S_u to $S_u^{+\perp} \cap \partial B_t(S_u)$. Hence, we obtain

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1+C\rho_\varepsilon)^3 \int_{S_u} \int_{\delta_\varepsilon}^{\rho_\varepsilon} \bigg(\frac{1}{\varepsilon}(W^2\circ\sigma_\varepsilon)\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nu_u,x+t\nu_u)}\Big) + \frac{1}{\varepsilon}\Big|\sigma_\varepsilon'\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nu_u,x+t\nu_u)}\Big)\Big|^2\bigg) K(x)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

where we additionally used that K is Lipschitz and stricly positively bounded from below. Applying that $x \mapsto \tilde{\varphi}(\nu, x)$ is Lipschitz together with W being decreasing and σ_ε being increasing we obtain

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1+C\rho_\varepsilon)^3 \int_{S_u} \int_{\delta_\varepsilon}^{\rho_\varepsilon} \bigg(\frac{1}{\varepsilon}(W^2\circ\sigma_\varepsilon)\Big(\frac{t}{\varepsilon(\tilde{\varphi}_2(\nu_u,x)+C\rho_\varepsilon)}\Big) + \frac{1}{\varepsilon}\Big|\sigma_\varepsilon'\Big(\frac{t}{\varepsilon(\tilde{\varphi}_2(\nu_u,x)+C\rho_\varepsilon)}\Big)\Big|^2\bigg) K(x)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}(x)\,,$$

Another change of variables, namely $t \mapsto t\varepsilon(\tilde{\varphi}_2(\nu_u, x) + C\rho_\varepsilon)$, and integrating over the whole interval where the integrand is non-zero yields

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1+C\rho_\varepsilon)^4 \int_{\tilde{\delta}_\varepsilon}^{\sigma^{-1}\left(\frac{1}{1+\gamma_\varepsilon}\right)+\tilde{\delta}_\varepsilon} \Big(W^2(\sigma_\varepsilon(t)) + |\sigma_\varepsilon'(t)|^2\Big)\,\mathrm{d}t \times \int_{S_u} \varphi_2(\nu_u,x)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

From the definitions one can easily check that on the integration domain we have $\sigma_\varepsilon = (1+\gamma_\varepsilon)\sigma(\cdot - \tilde{\delta}_\varepsilon)$ and $\sigma_\varepsilon' = (1+\gamma_\varepsilon)W(\sigma(\cdot - \tilde{\delta}_\varepsilon))$ so that

$$\mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le (1+C\rho_\varepsilon)^4(1+\gamma_\varepsilon)^2 \int_0^{\sigma^{-1}\left(\frac{1}{1+\gamma_\varepsilon}\right)} \Big(W^2((1+\gamma_\varepsilon)\sigma(t)) + W^2(\sigma(t))\Big)\,\mathrm{d}t \times \int_{S_u} \varphi_2(\nu_u,x)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

Using again that $W\circ\sigma$ is decreasing, we can simply compute

$$\int_0^{\sigma^{-1}\left(\frac{1}{1+\gamma_\varepsilon}\right)} \Big(W^2((1+\gamma_\varepsilon)\sigma(t)) + W^2(\sigma(t))\Big)\,\mathrm{d}t \le 2\int_0^\infty W^2(\sigma(t))\,\mathrm{d}t$$

$$= 2\int_0^\infty W(\sigma(t))\sigma'(t)\,\mathrm{d}t$$
$$= 2\int_0^1 W(t)\,\mathrm{d}t = 2c_W\,.$$

Therefore, we obtain from the previous estimations

$$\limsup_{\varepsilon\to 0} \mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon) \le 2c_W \int_{S_u} \varphi_2(\nu_u, x)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

We can repeat all the arguments for $G_\varepsilon|_{S_u^{-\perp}}(v_\varepsilon)$ with $\nabla\tau(x) = -\nu_u$ on $S_u^{-\perp}$. We consequently get

$$\limsup_{\varepsilon\to 0}\Big(\mathcal{G}_\varepsilon|_{S_u^{-\perp}}(v_\varepsilon) + \mathcal{G}_\varepsilon|_{S_u^{+\perp}}(v_\varepsilon)\Big) \le 4c_W \int_{S_u} \varphi_2(\nu_u, x)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,.$$

Next, we show that $\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp} \to 0$ as $\varepsilon \to 0$. For $x \in \Omega\setminus\overline{S_u}$ one can show that

$$\Big|\nabla\big[x \mapsto \tilde\varphi_2(\tau(x), x)\big]\Big| \le \frac{C}{\tau(x)}\,. \tag{4.22}$$

Indeed, let $x, y \in \Omega\setminus\overline{S_u}$ and assume without loss of generality that $\tau(x) \le \tau(y)$. From Lemma 2.1.1 we infer that $x = \pi_{S_u}(x) + \tau(x)\nabla\tau(x)$, where $\pi_{S_u}(x)$ denotes the projection of x onto S_u. Since the projection on a convex set is Lipschitz continuous with Lipschitz constant one (see e.g. [80, (3.1.4)]), for $\tilde y = \pi_{S_u}(y) + \tau(x)\nabla\tau(y)$, being the projection of y onto $B_{\tau(x)}(S_u)$, we have $|x - \tilde y| \le |x - y|$, and therefore

$$\big|\nabla\tau(x) - \nabla\tau(y)\big| = \frac{1}{\tau(x)}\Big|x - \pi_{S_u}(x) - (\tilde y - \pi_{S_u}(y))\Big| \le \frac{2}{\tau(x)}|x - y|\,. \tag{4.23}$$

Together with Assumption 4.1.1 (c) and (d) there holds for $x \in B_{\rho_\varepsilon}(S_u)$ and ε sufficiently small

$$\begin{aligned}\Big|\tilde\varphi_2(\nabla\tau(x), x) - \tilde\varphi_2(\nabla\tau(y), y)\Big| &\le C\big|\nabla\tau(x) - \nabla\tau(y)\big| + C|x - y| \\ &\le \frac{C}{\tau(x)}|x - y|\,,\end{aligned}$$

which yields (4.22). From (4.21) we therefore obtain

$$\tilde\varphi_2^2(\nabla v_\varepsilon(x), x) \le \frac{C}{\varepsilon^2}\Big|\sigma_\varepsilon'\Big(\frac{\tilde\tau(x)}{\varepsilon}\Big)\Big|^2 \quad \text{for all } x \in \Omega\setminus S_u^\perp\,.$$

We plug this in and apply as before the coarea formula in order to obtain

$$\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp}(v_\varepsilon) \le C\int_{\delta_\varepsilon}^{\rho_\varepsilon}\int_{\partial B_t(S_u)\setminus S_u^\perp}\Bigg(\frac{1}{\varepsilon}(W^2\circ\sigma_\varepsilon)\Big(\frac{t}{\varepsilon\tilde\varphi_2(\nabla\tau(x), x)}\Big)$$

$$+ \frac{1}{\varepsilon}\Big|\sigma_\varepsilon'\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nabla\tau(x),x)}\Big)\Big|^2\Big)K(x)\,\mathrm{d}\mathcal{H}^{n-1}(x)\,\mathrm{d}t\,.$$

Next, we use the coordinate transformation $x \mapsto x + (t-\delta_\varepsilon)\nabla\tau(x)$, which maps $\partial B_{\delta_\varepsilon}(S_u)$ onto $\partial B_t(S_u)$. Note, that $\nabla\tau(x) = \nabla\tau(x + t\nabla\tau(x))$ and from (4.23) we infer that $\|\nabla^2\tau\|_{L^\infty(\Omega\setminus S_u)} \le \frac{C}{\delta_\varepsilon}$ so that the coarea factor is bounded by $\frac{C\rho_\varepsilon}{\delta_\varepsilon}$. Hence, we get

$$\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp}(v_\varepsilon) \le \frac{C\rho_\varepsilon}{\delta_\varepsilon}\int_{\partial B_{\delta_\varepsilon}(S_u)\setminus S_u^\perp}\int_0^{\rho_\varepsilon-\delta_\varepsilon}\Big((W^2\circ\sigma_\varepsilon)\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nabla\tau(x),x+t\nabla\tau(x))}\Big)$$
$$+\Big|\sigma_\varepsilon'\Big(\frac{t}{\varepsilon\tilde{\varphi}_2(\nabla\tau(x),x+t\nabla\tau(x))}\Big)\Big|^2\Big)K(x)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}(x)\,,$$

where we again used the Lipschitz continuity and the uniform strictly positive bound of K, and additionally shifted the integral with respect to t. Repeating the same arguments used for the estimate of $\mathcal{G}_\varepsilon|_{S_u^{+\perp}}$ we get

$$\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp}(v_\varepsilon) \le \frac{C\rho_\varepsilon}{\delta_\varepsilon}c_W\int_{\partial B_{\delta_\varepsilon}(S_u)\setminus S_u^\perp}\varphi_2(\nabla\tau(x),x)\sqrt{K(x)}\,\mathrm{d}\mathcal{H}^{n-1}(x)\,,$$

Since φ_2 and K are uniformly bounded we obatin

$$\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp}(v_\varepsilon) \le \frac{C\rho_\varepsilon}{\delta_\varepsilon}\mathcal{H}^{n-1}(\partial B_{\delta_\varepsilon}(S_u)\setminus S_u^\perp)$$

It is easy to see that $\partial B_{\delta_\varepsilon}(S_u)\setminus S_u^\perp \subset \partial B_{\delta_\varepsilon}(\partial S_u)$, where ∂S_u denotes the relative boundary of S_u in the hyperplane $\nu_u^\perp$. Hence,

$$\mathcal{G}_\varepsilon|_{\Omega\setminus S_u^\perp}(v_\varepsilon) \le \frac{C\rho_\varepsilon}{\delta_\varepsilon}\mathcal{H}^{n-1}(\partial B_{\delta_\varepsilon}(\partial S_u)) \le C\rho_\varepsilon \to 0 \quad \text{as } \varepsilon\to 0\,.$$

Summing up, we conclude with (4.20) and the proof is complete. □

We close this section with a remark which slighlty generalizes our result.

Remark 4.1.6. In the setting of Teorem 4.1.2 we can split the functionals F_ε in the *elastic energy* defined on $L^1(\Omega)\times L^1(\Omega)$ by

$$\mathcal{E}_\varepsilon(u,v) := \begin{cases} \int_\Omega (f(v)+\eta_\varepsilon)\varphi_1^2(\nabla u,x)\,\mathrm{d}x & \text{for } u\in H^1(\Omega), v\in H^1(\Omega;[0,1]) \\ +\infty & \text{otherwise,}\end{cases}$$

and the *dissipative energy* defined by

$$\mathcal{D}_\varepsilon(u,v) := \begin{cases} \int_\Omega \frac{1}{\varepsilon}W^2(v)K + \varepsilon\varphi_2^2(\nabla v,x)\,\mathrm{d}x & \text{for } u\in H^1(\Omega), v\in H^1(\Omega;[0,1]) \\ +\infty & \text{otherwise}\end{cases}$$

Therefore, we have $F_\varepsilon(u,v) = \mathcal{E}_\varepsilon(u,v) + \mathcal{D}_\varepsilon(u,v)$ for all $u, v \in L^1(\Omega)$ In the same way we can write $F(u,v) = \mathcal{E}(u,v) + \mathcal{D}(u,v)$ for all $u, v \in L^1(\Omega)$ defining

$$\mathcal{E}(u,v) \begin{cases} \int_\Omega f(1)\varphi_1^2(\nabla u, x)\,\mathrm{d}x & \text{for } u \in \mathrm{GSBV}^2(\Omega), v = 1 \\ +\infty & \text{otherwise,} \end{cases}$$

and

$$\mathcal{D}(u,v) := \begin{cases} 4c_W \int_{S_u} \varphi_2^2(\nu_u, x)\sqrt{K}\,\mathrm{d}\mathcal{H}^{n-1}(x) & \text{for } u \in \mathrm{GSBV}^2(\Omega), v = 1 \\ +\infty & \text{for } v \in L^1(\Omega) \setminus H^1(\Omega; [0,1]) \end{cases}$$

Following the proof of Proposition 4.1.3 and Proposition 4.1.4 carefully we can infer that $\Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{E}_\varepsilon = \mathcal{E}$ and $\Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{D}_\varepsilon = \mathcal{D}$ under the assumption that F_ε is uniformly bounded. The corresponding lim sup-inequality follows directly from Proposition 4.1.5, so that (assuming F_ε is uniformly bounded) we obtain the Γ-convergence of the elastic and dissipative energy separately, i.e. $\Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{E}_\varepsilon = E$ and $\Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{D}_\varepsilon = \mathcal{D}$.

4.2 Phase Field Models of Thin Elastic Shells

We apply the result from Theorem 4.1.2 to our model derived in Chapter 3, where φ_1 and φ_2 are quadratic forms. Going back to the notation therein, we precisely set

$$\varphi_1^2(\zeta, x) = \varphi_2^2(\zeta, x) = \zeta_\alpha a^{\alpha\beta}(x)\zeta_\beta \sqrt{a(x)} \quad \text{for } \zeta \in \mathbb{R}^n, x \in \omega\,.$$

Futhermore, we set $K = \sqrt{a}$ in order to obtain

$$\mathcal{F}_\varepsilon(u,v) := \frac{1}{2}\int_\omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a}\,\mathrm{d}x + \frac{\mu}{2}\int_\omega (f(v) + \eta_\varepsilon)\partial_\alpha u\, a^{\alpha\beta}\partial_\beta u \sqrt{a}\,\mathrm{d}x + \kappa \int_\omega \frac{1}{\varepsilon} W^2(v)\sqrt{a} + \varepsilon\,\partial_\alpha v\, a^{\alpha\beta}\partial_\beta v \sqrt{a}\,\mathrm{d}x$$

for $u \in H^1(\omega)$ and $v \in H^1(\omega; [0,1])$. As a norm induced by a scalar product φ_1 and φ_2 clearly fulfil Assumption 4.1.1 (c). Choosing W and f such that $c_W = \frac{1}{4}$ and $f(1) = 1$ we can apply Theorem 4.1.2 such that $\mathcal{F}_\varepsilon$ Γ-converges to

$$\mathcal{F}(u,v) := \frac{1}{2}\int_\omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a}\,\mathrm{d}x + \frac{\mu}{2}\int_\omega \partial_\alpha u\, a^{\alpha\beta}\,\partial_\beta u\,\sqrt{a}\,\mathrm{d}x + \kappa \int_{S_u} \sqrt{[\nu_u]_\alpha a^{\alpha\beta} [\nu_u]_\beta}\sqrt{a}\,\mathrm{d}x\,, \tag{4.24}$$

which is precisely our fracture model of thin elastic shells which we derived in Theorem 3.3.3. Note that this choice for φ_2, K is not unique. The result holds still true by choosing for instance $K = a$ and $\varphi_2^2(\zeta, x) = \zeta_\alpha a^{\alpha\beta}\zeta_\beta$. The setting above, however, seems to be the most natural one, as it leads to the transformed Ambrosio-Tortorelli functional, meaning that by coordinate transformation $\phi\colon \omega \to \Omega$, given from the previous chapter, one can write

$$\mathcal{F}(u,v) := \frac{1}{2}\int_{\phi(\omega)} \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} \left|u \circ \phi^{-1}\right|^2 \mathrm{d}x + \frac{\mu}{2}\int_{\phi(\omega)} \left|\nabla_\tau (u \circ \phi^{-1})\right|^2 \mathrm{d}x + \kappa \mathcal{H}^1(\phi(S_u))$$

where $\nabla_\tau u$ denotes the tangential gradient of u. This looks pretty like the classical Ambrosio-Tortorelli functional, but expressed directly on the surface $\phi(\omega)$, and taking the curvature term into account.

Setting $W(t) = \frac{1}{2}(1-t)$ and $f(t) = t^2$, we obtain the elliptic functional

$$\begin{aligned} \mathcal{F}_\varepsilon(u,v) := \frac{1}{2}\int_\omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a}\,\mathrm{d}x + \frac{\mu}{2}\int_\omega (v^2 + \eta_\varepsilon)\partial_\alpha u\, a^{\alpha\beta}\partial_\beta u \sqrt{a}\,\mathrm{d}x \\ + \kappa \int_\omega \frac{1}{4\varepsilon}(1-v)^2\sqrt{a} + \varepsilon\, \partial_\alpha v\, a^{\alpha\beta}\partial_\beta v \sqrt{a}\,\mathrm{d}x \end{aligned} \tag{4.25}$$

as an approximation of $\mathcal{F}$. In flat land, where we have $b_{\alpha\beta} = 0$ and $\varphi_1(\cdot,x)$, $\varphi_2(\cdot,x)$ being the Euclidean norm, this is precisely the standard Ambrosio-Tortorelli functional from (4.1). This choice will also be our standard choice for the following chapters, since the quadratic form, we obtain in this way, simplifies the numerical computations by leading to linear Euler-Lagrange equations.

Remark 4.2.1. Following Remark 4.1.6 we obtain that

$$\kappa \int_\omega \frac{1}{4\varepsilon}(1-v)^2\sqrt{a} + \varepsilon\, \partial_\alpha v\, a^{\alpha\beta}\partial_\beta v \sqrt{a}\,\mathrm{d}x$$

Γ-converges to

$$\kappa \int_{S_u} \sqrt{[\nu_u]_\alpha a^{\alpha\beta}[\nu_u]_\beta}\sqrt{a}\,\mathrm{d}x\,.$$

Hence, the crack length can be approximately measured by the functional

$$\frac{1}{\kappa}\mathcal{D}_\varepsilon(v) = \int_\omega \frac{1}{4\varepsilon}(1-v)^2\sqrt{a} + \varepsilon\, \partial_\alpha v\, a^{\alpha\beta}\partial_\beta v \sqrt{a}\,\mathrm{d}x$$

4.3 Approximation by Phase Fields of Bounded Variation

In this section we present an approximation of the Mumford-Shah functional similar to the one of Ambrosio and Tortorelli, but this time allowing the phase field variable v to be a function of bounded variation. This represents in some sense the case in (4.2) with $p = 1$.

For our main result we need several, quite technical assumptions. In order to keep a better overview we first list them here.

Assumption 4.3.1. Let $\varepsilon_0 > 0$. For each $0 < \varepsilon < \varepsilon_0$ let

(a) $W_\varepsilon\colon [0,1] \to [0,\infty)$ be continuous such that $W_\varepsilon \to W$ in $L^1([0,1])$ as $\varepsilon \to 0$ for some $W \in L^1([0,1])$, with $1 \in \operatorname{ess\,supp} W$, and $W_\varepsilon \leq \int_0^1 W(s)\,\mathrm{d}s$ a.e. in $[0,1]$.

(b) $\varphi_\varepsilon\colon W_\varepsilon([0,1]) \to \mathbb{R}$ be a convex function such that $\varphi_\varepsilon(W_\varepsilon(1)) \to 0$ and $\varphi_\varepsilon(W_\varepsilon(\cdot)) \to +\infty$ uniformly on $[0,T]$ for all $0 < T < 1$, i.e. for all $C > 0$ there exists $0 < \tilde{\varepsilon} < \varepsilon_0$ such that $\varphi_\varepsilon(W_\varepsilon(t)) > C$ for all $t \in [0,T]$ and $\varepsilon < \tilde{\varepsilon}$.

(c) $\psi_\varepsilon\colon [0,\infty) \to \mathbb{R}$ be an increasing function such that $\psi_\varepsilon(0) \to 0$ as $\varepsilon \to 0$ and $\varphi_\varepsilon^* \leq \psi_\varepsilon$ on $[0,\infty)$, where φ_ε^* denotes the convex conjugate of φ_ε (see Section 2.2).

(d) $\eta_\varepsilon \geq 0$ such that $\eta_\varepsilon \varphi_\varepsilon(W_\varepsilon(0)) \to 0$ as $\varepsilon \to 0$.

Furthermore, assume that

(e) $f\colon [0,1] \to [0,\infty)$ is a continuous, non-decreasing function with $f(0) = 0$ and $f > 0$ on $(0,1]$.

We are now ready to state our main theorem.

Theorem 4.3.2. *Let $\Omega \subset \mathbb{R}^n$ be a non-empty, open, bounded set with Lipschitz boundary, let W_ε, φ_ε, ψ_ε, η_ε and f be given as in Assumption 4.3.1, and let $c_W = \int_0^1 W(s)\,\mathrm{d}s$. For each $\varepsilon > 0$, we define the functional $F_\varepsilon\colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by*

$$F_\varepsilon(u,v) := \int_\Omega (f(v) + \eta_\varepsilon)|\nabla u|^2 + \varphi_\varepsilon(W_\varepsilon(v)) + \psi_\varepsilon(|\nabla v|)\,\mathrm{d}x + c_W\big(|\mathrm{D}^j v|(\Omega) + |\mathrm{D}^c v|(\Omega)\big) \tag{4.26}$$

for all $u \in H^1(\Omega), v \in \mathrm{BV}(\Omega;[0,1])$ and $F_\varepsilon(u,v) := +\infty$ otherwise.

Moreover, define $F\colon L^1(\Omega) \times L^1(\Omega) \to \mathbb{R}$ by

$$F(u,v) := \begin{cases} \displaystyle\int_\Omega f(1)|\nabla u|^2\,\mathrm{d}x + 2c_W\mathcal{H}^{n-1}(S_u) & \text{for } u \in \mathrm{GSBV}^2(\Omega), v = 1 \text{ a.e.},\\ +\infty & \text{otherwise}. \end{cases}$$

Then there holds $F = \Gamma\text{-}\lim_{\varepsilon\to 0} F_\varepsilon$.

The following corollary represents a special case of the previous theorem, and represents our actual main result of this paper. Based on this we perform our numerical computations in Section 4.4.

Corollary 4.3.3. *Let $\Omega \subset \mathbb{R}^n$ be a non-empty, open, bounded set with Lipschitz boundary. For each $\varepsilon > 0$ let $\eta_\varepsilon > 0$ such that $\frac{\eta_\varepsilon}{\varepsilon} \to 0$ as $\varepsilon \to 0$ and define the functional*

$$F_\varepsilon(u,v) := \frac{\alpha}{2}\int_\Omega (v^2 + \eta_\varepsilon)|\nabla u|^2\,\mathrm{d}x + \frac{\gamma}{2\varepsilon}\int_\Omega (1-v)\,\mathrm{d}x + \frac{\gamma}{2}|\mathrm{D}v|(\Omega)$$

if $u \in H^1(\Omega), v \in \mathrm{BV}(\Omega;[0,1])$ *and* $F_\varepsilon(u,v) := +\infty$ *otherwise. Moreover, define* $F\colon L^1(\Omega)\times L^1(\Omega)\to\mathbb{R}$ *by*

$$F(u,v) := \begin{cases} \frac{\alpha}{2}\int_\Omega |\nabla u|^2\,\mathrm{d}x + \gamma\mathcal{H}^{n-1}(S_u) & \text{for } u\in \mathrm{GSBV}^2(\Omega), v=1 \text{ a.e.}\,,\\ +\infty & \text{otherwise.}\end{cases}$$

Then there holds $F = \Gamma\text{-}\lim_{\varepsilon\to 0} F_\varepsilon$.

Proof of Corollary 4.3.3. We define $\tilde F_\varepsilon := \frac{2}{\gamma}F_\varepsilon$ and, choose the functions f, W_ε, φ_ε and ψ_ε in the following way:

$$f(t) = \frac{\alpha}{\gamma}t^2, \qquad W_\varepsilon(t) = (1-t)^\varepsilon, \qquad \varphi_\varepsilon(t) = \frac{1}{\varepsilon}t^{\frac{1}{\varepsilon}}, \qquad \psi_\varepsilon(s) = s$$

for all $t\in[0,1], s\in[0,\infty)$ and $0<\varepsilon<1$. Note that in this setting we have

$$\varphi_\varepsilon^*(s) = \begin{cases}(1-\varepsilon)(\varepsilon^{2\varepsilon}s)^{\frac{1}{1-\varepsilon}} & \text{for } s\in[0,\varepsilon^{-2}]\,,\\ s-\frac{1}{\varepsilon} & \text{for } s>\varepsilon^{-2}\,,\end{cases}$$

and hence, one can simply verify that Assumption 4.3.1 is fulfilled with $W = \mathbb{1}$, the constant one function.

From Theorem 4.3.2 we get that $\tilde F_\varepsilon$ Γ-converges to

$$\tilde F(u,v) := \begin{cases} \frac{\alpha}{\gamma}\int_\Omega |\nabla u|^2\,\mathrm{d}x + 2\mathcal{H}^{n-1}(S_u) & \text{for } u\in \mathrm{GSBV}^2(\Omega), v=1 \text{ a.e.}\\ +\infty & \text{otherwise.}\end{cases}$$

Since Γ-convergence is preserved under constant multiplication we get the result by multiplying $\tilde F_\varepsilon$ and $\tilde F$ with $\frac{\gamma}{2}$. □

Remark 4.3.4. We remark once more that since Γ-convergence is stable under continuous perturbations we simply get that

$$\Gamma\text{-}\lim_{\varepsilon\to 0}\Big(F_\varepsilon + \beta\int_\Omega |\cdot - g|^2\,\mathrm{d}x\Big) = F + \beta\int_\Omega |\cdot - g|^2\,\mathrm{d}x\,.$$

Since Theorem 4.3.2 and thus Corollary 4.3.3 also holds true for $\eta_\varepsilon = 0$, we can omit this parameter in our numerical computations. However, the minimization of only F_ε becomes an ill-posed problem when $v=0$ on a set of non-zero measure. Therefore, in order to make our results applicable to fracture mechanics, we take the case for $\eta_\varepsilon>0$ also into account.

The proof of Theorem 4.3.2 follows the usual strategy that has been used for the classical Ambrosio-Tortorelli approximation and various generalizations (see [12, 13, 34, 56, 82, 83]). Firstly, we show the lim inf-inequality on the real line (see Proposition 4.3.5).

The generalization to the multi-dimensional case, stated in Proposition 4.3.6, is then shown by a slicing argument.

The lim sup-inequality is again shown with the help of the density result in $\mathrm{SBV}^2(\Omega)\cap L^\infty(\Omega)$ (see Theorem 2.4.1). Here, we exploit the fact that the phase field variable is allowed to have jumps, which enables the construction of a much simpler recovery sequence than when the phase field needs to be smooth.

Proposition 4.3.5. *In the setting of Theorem 4.3.2 with $\Omega \subset \mathbb{R}$ we redefine $F\colon L^1(\Omega)\times L^1(\Omega) \to \mathbb{R}$ by*

$$F(u,v) := \begin{cases} \int_\Omega f(1)|u'|^2 \,\mathrm{d}x + 2c_W \# S_u & \text{for } u \in \mathrm{SBV}^2(\Omega), v = 1 \text{ a.e.} \\ +\infty & \text{otherwise} \end{cases}$$

Then there holds $F \leq \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon$.

Proof. First of all, for each open set $I \subset \Omega$ we define the localized functionals

$$F_\varepsilon(u,v;I) := \int_I (f(v)+\eta_\varepsilon)|u'|^2 + \varphi_\varepsilon(W_\varepsilon(v)) + \psi_\varepsilon(|v'|)\,\mathrm{d}x \\ + c_W\left(|\mathrm{D}^j v|(I) + |\mathrm{D}^c v|(I)\right)$$

for all $u \in H^1(I)$ and $v \in \mathrm{BV}(I;[0,1])$, and $F_\varepsilon(u,v;I) := +\infty$ otherwise.

Now, let (ε_j) be a sequence greater than zero with $\varepsilon_j \to 0$ as $j\to\infty$, and let (u_j) and (v_j) be sequences in $L^1(\Omega)$ such that $u_j \to u$ and $v_j \to v$ as $j \to \infty$. We can assume (up to a subsequence) that

$$\liminf_{j\to\infty} F_{\varepsilon_j}(u_j,v_j) = \lim_{j\to\infty} F_{\varepsilon_j}(u_j,v_j) < \infty\,.$$

Therefore, we must have $\int_\Omega \varphi_\varepsilon(W_\varepsilon(v_j))\,\mathrm{d}x < \infty$, and because of to the uniform convergence of $\varphi_\varepsilon(W_\varepsilon(\cdot))$ to $+\infty$ as $\varepsilon \to 0$ (see Assumption 4.3.1 (a)), we can assume that $v = 1$ a.e. on Ω.

We first show that $\# S_u$ is finite and

$$2c_W \# S_u \leq \liminf_{j\to\infty} F_{\varepsilon_j}(u_j,v_j;B_\delta(S_u)) \quad \text{for all } \delta > 0 \text{ sufficiently small}\,. \tag{4.27}$$

For that let $y_0 \in S_u$, and let $\delta > 0$ sufficiently small such that $B_\delta(y_0) \subset \Omega$. Set $M := \liminf_{j\to\infty} \operatorname{ess\,inf}_{B_{\frac{\delta}{2}}(y_0)}(f\circ v_j)$ and assume that $M > 0$. Furthermore, let $0 < \eta < M$ and choose $j_0 > 0$ such that up to subsequence there holds $M < \operatorname{ess\,inf}_{B_{\frac{\delta}{2}}(y_0)}(f\circ v_j) + \eta$ for all $j > j_0$. Then there holds

$$\int_{y_0-\frac{\delta}{2}}^{y_0+\frac{\delta}{2}} |u_j'|^2\,\mathrm{d}x \leq \frac{1}{M-\eta}\int_{y_0-\frac{\delta}{2}}^{y_0+\frac{\delta}{2}} f(v_j)|u_j'|^2\,\mathrm{d}x \leq \frac{C}{M-\eta} \quad \text{for all } j > j_0$$

so that u_j' converges weakly to u' in $L^2(B_{\frac{\delta}{2}}(y_0))$ and consequently $y_0 \notin S_u$. Hence, we must have $M = 0$, and we can find a sequence (y_j) such that $f(\tilde{v}_j(y_j)) \to 0$, where $\tilde{v}_j$ is a precise representative of v_j. The assumptions on f in Assumption 4.3.1 (e) imply $\tilde{v}_j(y_j) \to 0$ as $j \to \infty$. Since $\tilde{v}_j \to 1$ a.e. we can, therefore, find $y^+, y^- \in B_\delta(y_0)$ with $y^- < y_0 < y^+$ such that $\tilde{v}_j(y^-) \to 1$ as well as $\tilde{v}_j(y^+) \to 1$.

With this at hand we get from the L^1-convergence of W_ε (see Assumption 4.3.1 (a)),

$$2c_W = \lim_{j\to\infty} \left[\int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^+)} W_{\varepsilon_j}(s)\,\mathrm{d}s + \int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^-)} W_{\varepsilon_j}(s)\,\mathrm{d}s \right]. \tag{4.28}$$

Defining

$$\Phi_\varepsilon(t) := \int_0^t W_\varepsilon(s)\,\mathrm{d}s \quad \text{for all } t \in [0,1], \varepsilon > 0$$

we get

$$\begin{aligned}\int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^+)} W_{\varepsilon_j}(s)\,\mathrm{d}s &+ \int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^-)} W_{\varepsilon_j}(s)\,\mathrm{d}s \\ &= \left|\Phi_{\varepsilon_j}(\tilde{v}_j(y^+)) - \Phi_{\varepsilon_j}(\tilde{v}_j(y_j))\right| + \left|\Phi_{\varepsilon_j}(\tilde{v}_j(y^-)) - \Phi_{\varepsilon_j}(\tilde{v}_j(y_j))\right|\end{aligned}$$

and together with (2.4)

$$\int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^+)} W_{\varepsilon_j}(s)\,\mathrm{d}s + \int_{\tilde{v}_j(y_j)}^{\tilde{v}_j(y^-)} W_{\varepsilon_j}(s)\,\mathrm{d}s \le \left|\mathrm{D}(\Phi_{\varepsilon_j} \circ v_j)\right|(B_\delta(y_0)). \tag{4.29}$$

Applying the chain rule (see (2.5)) and Fenchel's inequality (see (2.1)) yields

$$\begin{aligned}&\left|\mathrm{D}(\Phi_{\varepsilon_j} \circ v_j)\right|(B_\delta(y_0)) \\ &= \int_{y_0-\delta}^{y_0+\delta} W_{\varepsilon_j}(v_j)|v_j'|\,\mathrm{d}x \\ &\quad + \int_{J_{v_j}\cap B_\delta(y_0)} \left|\Phi_{\varepsilon_j}(v_j^+) - \Phi_{\varepsilon_j}(v_j^-)\right|\mathrm{d}\mathcal{H}^0 + \int_{B_\delta(y_0)} \Phi'(\tilde{v}_j)\,\mathrm{d}|\mathrm{D}^c v_j| \\ &\le \int_{y_0-\delta}^{y_0+\delta} \varphi_\varepsilon(W_{\varepsilon_j}(v_j)) + \varphi_\varepsilon^*(|v_j'|)\,\mathrm{d}x \\ &\quad + \int_{J_{v_j}\cap B_\delta(y_0)} \int_{v_j^-}^{v_j^+} W_{\varepsilon_j}(s)\,\mathrm{d}s\,\mathrm{d}\mathcal{H}^0 + \int_{B_\delta(y_0)} W_{\varepsilon_j}(\tilde{v}_j)\,\mathrm{d}|\mathrm{D}^c v_j| \\ &\le F_{\varepsilon_j}(u_j, v_j; B_\delta(y_0)).\end{aligned} \tag{4.30}$$

In the last inequality we used $\varphi_\varepsilon^* \le \psi_\varepsilon$ on $[0,\infty)$ from Assumption 4.3.1 (c) and $W_{\varepsilon_j} \le c_W$ from Assumption 4.3.1 (a). By merging (4.28), (4.29) and (4.30) we deduce

$$2c_W \le \liminf F_{\varepsilon_j}(u_j, v_j; B_\delta(y_0)).$$

For each $N \leq \#S_u$ we can repeat the preceding arguments for each element in a set $\{y_1, \dots, y_N\} \subset S_u$ with $\delta > 0$ sufficiently small such that $B_\delta(y_k) \cap B_\delta(y_\ell) = \emptyset$ for $k \neq \ell$ in order to obtain

$$2c_W N \leq \sum_{k=1}^{N} \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; B_\delta(y_k)) \leq \liminf_{j\to\infty} F_{\varepsilon_j}\left(u_j, v_j; \bigcup_{k=1}^{N} B_\delta(y_k)\right).$$

By assumption the right hand side is finite; hence, there must hold $\#S_u < \infty$ and we deduce (4.27).

In the next step we show that for all $\delta > 0$

$$\int_{\Omega\setminus B_\delta(S_u)} f(1)|u'|^2 \,\mathrm{d}x \leq \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; \Omega \setminus \overline{B_\delta(S_u)}). \tag{4.31}$$

Let $I := (a, b) \subset \Omega$ be an open interval such that $I \cap S_u = \emptyset$. For $k \in \mathbb{N}$ and $\ell \in \{1, \dots, k\}$ we define the intervals

$$I_\ell^k := \left(a + \frac{\ell - 1}{k}(b-a), a + \frac{\ell}{k}(b-a)\right)$$

and we extract a subsequence of (v_j) (not relabeled) such that $\lim_{j\to\infty} \operatorname{ess\,inf}_{I_\ell^k} v_j$ exists for all ℓ. Moreover, for $0 < z < 1$ we define the set

$$T_z^k := \{\ell \in \{1, \dots, k\} \colon \lim_{j\to\infty} \operatorname*{ess\,inf}_{I_\ell^k} v_j \leq z\}.$$

For any $\ell \in T_z^k$ there exists a sequence (x_j) in I_ℓ^k and $y \in I_\ell^k$ such that

$$\lim_{j\to\infty} \tilde{v}_j(x_j) = \lim_{j\to\infty} \operatorname*{ess\,inf}_{I_\ell^k} v_j \qquad \text{and} \qquad \tilde{v}_j(y) \to 1.$$

With this at hand we can estimate precisely as in (4.29) and (4.30)

$$\int_z^1 W(s)\,\mathrm{d}s \leq \lim_{j\to\infty} \int_{\tilde{v}_j(x_j)}^{\tilde{v}_j(y)} W_{\varepsilon_j}(s)\,\mathrm{d}s \leq \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; I_\ell^k) \leq C$$

for some $C > 0$ by assumption.

Repeating this argument for every $\ell \in T_z^k$ we get

$$\#(T_z^k) \int_z^1 W(s)\,\mathrm{d}s \leq \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; I) \leq C.$$

Note that, since $1 \in \operatorname{ess\,supp} W$ from Assumption 4.3.1 (a), there holds $\int_z^1 W(s)\,\mathrm{d}s > 0$ for all $0 < z < 1$ and hence, $\#T_z^k$ is bounded independently of k. Because $\#T_z^k$ is non-decreasing with respect to k, for k large enough we can pick $\ell_1^k < \ell_2^k < \cdots < \ell_N^k \in T_z^k$ with $N = \max_{k\in\mathbb{N}} \#(T_z^k)$, such that each $\frac{\ell_i^k}{k}$ converges to some $y_i \in \bar{I}$ as $k \to \infty$. Define

$T_z = \{y_1, \dots, y_N\}$, let $\delta > 0$, and choose $k > \frac{b-a}{2\delta}$ and $\ell \in T_z^k$. Then we have $I_\ell^k \subset B_\delta(T_z)$. Therefore,

$$\liminf_{j\to\infty} f(z) \int_{I\setminus B_\delta(T_z)} |u_j'|^2 \, \mathrm{d}x \le \liminf_{j\to\infty} \int_I f(v_j)|u_j'|^2 \, \mathrm{d}x \le \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; I) .$$

Since $\delta > 0$ was chosen arbitrarily it is possible to integrate over $I \setminus T_z$ on the left hand side. Moreover, from Assumption 4.3.1 (e) we have $f(z) > 0$, and thus, we obtain $u_j' \rightharpoonup u'$ in $L^2(I \setminus T_z)$ up to a subsequence, and consequently $u \in H^1(I \setminus T_z)$. Since $I \cap S_u = \emptyset$ there even holds $u \in H^1(I)$. Letting $z \to 1$ and using the weak lower semi-continuity of the norm as well as the continuity of f from Assumption 4.3.1 (e) we get

$$\int_I f(1)|u'|^2 \, \mathrm{d}x \le \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j; I) .$$

Since $I \subset \Omega$ was chosen arbitrarily such that $I \cap S_u = \emptyset$ we conclude (4.31). Together with (4.27) we eventually obtain $F(u, v) \le \liminf_{j\to\infty} F_{\varepsilon_j}(u_j, v_j)$. □

Proposition 4.3.6. *In the setting of Theorem 4.3.2 there holds*

$$F(u, v) \le \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon(u, v) \quad \textit{for all } u, v \in L^1(\Omega) .$$

Proof. For the proof we use the usual notation in the setting of slicing, introduced in Section 2.4. In what follows let $A \subset \Omega$ be open, $\xi \in \mathbb{S}^{n-1}$ and $y \in A_\xi$. Furthermore, let $u, v \in L^1(\Omega)$ be chosen arbitrarily. We define the localized version of (4.26) by

$$F_\varepsilon(u, v; A) := \int_A (f(v) + \eta_\varepsilon)|\nabla u|^2 + \varphi_\varepsilon(W_\varepsilon(v)) + \psi_\varepsilon(|\nabla v|) \, \mathrm{d}x \\ + c_W (|\mathrm{D}^j v|(A) + |\mathrm{D}^c v|(A))$$

if $u \in H^1(A), v \in \mathrm{BV}(A; [0, 1])$ and $F_\varepsilon(u, v; A) := +\infty$ otherwise. Furthermore, we define for $I \subset \mathbb{R}$ open

$$F_\varepsilon^{\xi,y}(u, v; I) := \int_I (f(v) + \eta_\varepsilon)|u'|^2 + \varphi_\varepsilon(W_\varepsilon(v)) + \psi_\varepsilon(|v'|) \, \mathrm{d}x \\ + c_W (|\mathrm{D}^j v|(I) + |\mathrm{D}^c v|(I))$$

if $u \in H^1(I), v \in \mathrm{BV}(I; [0, 1])$ and $F_\varepsilon^{\xi,y}(u, v; I) := +\infty$ otherwise. We additionally set

$$F_\varepsilon^\xi(u, v; A) := \int_{A_\xi} F_\varepsilon^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi) \mathrm{d}\mathcal{L}^{n-1}(y) .$$

From Fubini's theorem and Theorem 2.4.2 we therefore obtain

$$F_\varepsilon^\xi(u, v; A) = \int_A (f(v) + \eta_\varepsilon)\big|\langle \nabla u, \xi\rangle\big|^2 + \varphi_\varepsilon(W_\varepsilon(v)) + \psi_\varepsilon(|\langle \nabla v, \xi\rangle|) \, \mathrm{d}x \\ + c_W \big|\langle \mathrm{D}^j v, \xi\rangle\big|(A) + c_W \big|\langle \mathrm{D}^c v, \xi\rangle\big|(A)$$

if $|\langle \mathrm{D}u, \xi\rangle|$ is absolutely continuous with respect to $\mathcal{L}^n$, and $F_\varepsilon^\xi(u, v; A) = +\infty$ otherwise. Thus, there clearly holds

$$F_\varepsilon^\xi(u, v; A) \leq F_\varepsilon(u, v; A)\,.$$

From Proposition 4.3.5 we know that

$$F^{\xi,y}(u, v; I) \leq \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon^{\xi,y}(u, v; I)$$

with

$$F^{\xi,y}(u, v; I) := \begin{cases} \displaystyle\int_I f(1)|u'|^2 \,\mathrm{d}x + 2c_W \# S_u & \text{for } u \in \mathrm{SBV}^2(I), v = 1 \text{ a.e.,} \\ +\infty & \text{otherwise.} \end{cases}$$

Choosing

$$F^\xi(u, v; A) := \int_{A_\xi} F^{\xi,y}(u_y^\xi, v_y^\xi; A_y^\xi) \,\mathrm{d}\mathcal{L}^{n-1}(y)\,,$$

we obtain in the same way as we have achieved (4.12) in the proof of Proposition 4.1.4

$$F^\xi(u, v; A) \leq \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon^\xi(u, v; A) \leq \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon(u, v; A)\,. \tag{4.32}$$

Furthermore, by following the lines of the proof of Proposition 4.1.4 we get that

$$F^\xi(u, v; A) = \int_A f(1)|\langle \nabla u, \xi\rangle|^2 \,\mathrm{d}x + 2c_W \int_{S_u} |\langle \nu_u, \xi\rangle| \,\mathrm{d}\mathcal{H}^{n-1}$$

if $u \in \mathrm{GSBV}^2(A)$ and $v = 1$ a.e. in A, and $F^\xi(u, v; A) = +\infty$ otherwise.

Since A and ξ were chosen arbitrarily, a localization argument (see e.g. [34, Theorem 1.16]) and (4.32) imply

$$\begin{aligned} F(u, v; A) &= \int_A f(1) \sup_{\xi\in\mathbb{S}^{n-1}} |\langle \nabla u, \xi\rangle|^2 \,\mathrm{d}\mathcal{L}^n + 2c_W \int_{S_u} \sup_{\xi\in\mathbb{S}^{n-1}} |\langle \nu_u, \xi\rangle| \mathcal{H}^{n-1} \\ &\leq \Gamma\text{-}\liminf_{\varepsilon\to 0} F_\varepsilon(u, v; A)\,, \end{aligned}$$

for $v = 1$ a.e. on A. Otherwise, the lim inf-inequality follows directly from (4.32) with ξ arbitrary. □

The following proposition now shows the lim sup-inequality.

Proposition 4.3.7. *In the setting of Theorem 4.3.2 there holds*

$$\Gamma\text{-}\limsup_{\varepsilon\to 0} F_\varepsilon(u, v) \leq F(u, v) \quad \textit{for all } u, v \in L^1(\Omega)\,.$$

Proof. If $u \notin \mathrm{GSBV}^2(\Omega)$ or $v \neq 1$ on some set with non-zero measure the assertion is obvious. We first show that the result holds for u replaced by $w \in \mathrm{SBV}^2(\Omega) \cap L^\infty(\Omega)$ for which ((a))–((c)) in Theorem 2.4.1 (replacing w_j by w) hold.

For this purpose choose for every $\varepsilon > 0$ some $\delta_\varepsilon > 0$ such that $\frac{\eta_\varepsilon}{\delta_\varepsilon} \to 0$ as $\varepsilon \to 0$ but still $\delta_\varepsilon \varphi_\varepsilon(W_\varepsilon(0)) \to 0$ as $\varepsilon \to 0$, for instance

$$\delta_\varepsilon = \frac{\sqrt{\eta_\varepsilon}}{\sqrt{\varphi_\varepsilon(W_\varepsilon(0))}}\,.$$

Take some smooth cutoff function $\phi\colon \mathbb{R} \to \mathbb{R}$ with $\phi = 1$ on $B_{\frac{1}{2}}(0)$ and $\phi = 0$ on $\Omega \setminus B_1(0)$, and define $\tau(x) = \operatorname{dist}(x, S_w)$ for all $x \in \Omega$. Then, we set $\phi_\varepsilon(x) = \phi(\tau(x)/\delta_\varepsilon)$ for all $x \in \Omega$, and we fix for every $\varepsilon > 0$ the function $w_\varepsilon = (1-\phi_\varepsilon)w$, for which holds $w_\varepsilon \in H^1(\Omega)$, $w_\varepsilon = w$ on $\Omega \setminus B_{\delta_\varepsilon}(S_w)$ and $w_\varepsilon \to w$ in $L^1(\Omega)$ as $\varepsilon \to 0$. Furthermore we define

$$v_\varepsilon = \begin{cases} 0 & \text{on } B_{\delta_\varepsilon}(S_w) \cap \Omega\,, \\ 1 & \text{elsewhere.} \end{cases}$$

Since $\overline{S_w}$ is polyhedral there holds $\mathcal{H}^{n-1}(\partial B_{\delta_\varepsilon}(S_w) \cap \Omega) < \infty$. Consequently, we have $v_\varepsilon \in \mathrm{BV}(\Omega; [0,1])$ for all $\varepsilon > 0$.

With this at hand, recalling Assumption 4.3.1 (e), we get

$$\begin{aligned} &F_\varepsilon(w_\varepsilon, v_\varepsilon) \\ &\le \int_\Omega f(1)|\nabla w|^2 \,\mathrm{d}x + \eta_\varepsilon \int_\Omega |\nabla w_\varepsilon|^2 \,\mathrm{d}x + \mathcal{L}^n(\Omega)\big(\varphi_\varepsilon(W_\varepsilon(1)) + \psi_\varepsilon(0)\big) \\ &\quad + \mathcal{L}^n(B_{\delta_\varepsilon}(S_w))\varphi_\varepsilon(W_\varepsilon(0)) + \mathcal{H}^{n-1}(\partial B_{\delta_\varepsilon}(S_w)) c_W\,. \end{aligned} \tag{4.33}$$

By the choice of w_ε, the fact that $\|w\|_{L^\infty(\Omega)} \le M$ and that $|\nabla \tau(x)| = 1$ for a.e. on Ω (see [62, Lemma 3.2.34]) we get on $B_{\delta_\varepsilon}(S_w)$

$$|\nabla w_\varepsilon| \le |w \nabla \phi_\varepsilon| + |(1-\phi_\varepsilon)\nabla w| \le \frac{M}{\delta_\varepsilon}\|\phi'\|_{L^\infty(\Omega)} + |\nabla w|\,,$$

which implies

$$\begin{aligned} &\eta_\varepsilon \int_\Omega |\nabla w_\varepsilon|^2 \,\mathrm{d}x \\ &\qquad \le \eta_\varepsilon \int_{\Omega \setminus B_{\delta_\varepsilon}(S_w)} |\nabla w|^2 \,\mathrm{d}x + C\frac{\eta_\varepsilon}{\delta_\varepsilon^2}\mathcal{L}^n(B_{\delta_\varepsilon}(S_w)) + 2\eta_\varepsilon \int_{B_{\delta_\varepsilon}(S_w)} |\nabla w|^2 \,\mathrm{d}x\,. \end{aligned}$$

with $C = 2M^2\|\phi'\|^2_{L^\infty(\Omega)}$ independent of ε. The first and the last term obviously converge to 0 as $\varepsilon \to 0$. For the second term we remark that for a polyhedral set, the Hausdorff measure coincides with the Minkowski content (see, e.g., [62, Theorem 3.2.29]), so that

$$\frac{\mathcal{L}^n(B_{\delta_\varepsilon}(\overline{S_w}))}{2\delta_\varepsilon} \to \mathcal{H}^{n-1}(\overline{S_w}) = \mathcal{H}^{n-1}(S_w) < \infty \quad \text{as } \varepsilon \to 0\,. \tag{4.34}$$

As a consequence, recalling that $\frac{\eta_\varepsilon}{\delta_\varepsilon} \to 0$ we get

$$C\frac{\eta_\varepsilon}{\delta_\varepsilon^2}\mathcal{L}^n\big(B_{\delta_\varepsilon}(S_w)\big) \to 0 \quad \text{as } \varepsilon \to 0\,,$$

and therefore

$$\eta_\varepsilon \int_\Omega |\nabla w_\varepsilon|^2 \,\mathrm{d}x \to 0 \quad \text{as } \varepsilon \to 0.$$

Additionally, (4.34) and $\delta_\varepsilon \varphi_\varepsilon(W_\varepsilon(0)) \to 0$ as $\varepsilon \to 0$ imply

$$\mathcal{L}^n\big(B_{\delta_\varepsilon}(S_w)\big)\varphi_\varepsilon(W_\varepsilon(0)) \to 0 \quad \text{as } \varepsilon \to 0\,.$$

Furthermore, there holds

$$\mathcal{H}^{n-1}\big(\partial B_{\delta_\varepsilon}(S_w)\big) \to 2\mathcal{H}^{n-1}(S_w) \quad \text{as } \varepsilon \to 0\,,$$

which is again due to $\overline{S_w}$ being a polyhedral set.

Applying the previous three convergence statements in (4.33) together with the limit behaviour of $\varphi_\varepsilon(W_\varepsilon(1))$ and $\psi_\varepsilon(0)$ from Assumption 4.3.1 (b) and (c), we get

$$\limsup_{\varepsilon\to 0} F_\varepsilon(w_\varepsilon, v_\varepsilon) \le F(w, \mathbb{1})\,. \tag{4.35}$$

Here, $\mathbb{1}$ represents the function that maps to 1 a.e. on Ω.

If $u \in \mathrm{GSBV}^2(\Omega)$ we have for every $M > 0$ that $u^M \in \mathrm{SBV}^2(\Omega) \cap L^\infty(\Omega)$ with $u^M := (-M) \vee u \wedge M$, and we can find a sequence (w_j) in $\mathrm{SBV}^2(\Omega) \cap L^\infty(\Omega)$ such that (a)–(f) in Theorem 2.4.1 (replacing u by u^M) holds. Together with the lower semi-continuity of $\Gamma\text{-}\limsup F_\varepsilon$ in $L^1(\Omega) \times L^1(\Omega)$ and (4.35) we deduce

$$\Gamma\text{-}\limsup_{\varepsilon\to 0} F_\varepsilon(u^M, \mathbb{1}) \le \liminf_{j\to\infty} \Gamma\text{-}\limsup_{\varepsilon\to 0} F_\varepsilon(w_j, \mathbb{1}) \le \liminf_{j\to\infty} F(w_j, \mathbb{1}) = F(u^M, \mathbb{1})\,.$$

Since $\nabla u \in L^2(\Omega)$ we get by the dominated convergence theorem

$$\lim_{M\to\infty} \int_\Omega \left|\nabla u^M\right|^2 \mathrm{d}x \to \int_\Omega |\nabla u|^2 \,\mathrm{d}x\,.$$

From $S_u = \bigcup_{M>0} S_{u^M}$ (see Section 2.4) follows that $\mathcal{H}^{n-1}(S_{u^M}) \le \mathcal{H}^{n-1}(S_u)$. Thus, using again the lower semi-continuity of $\Gamma\text{-}\limsup F_\varepsilon$ we conclude the proof letting $M \to \infty$. □

The proof of Theorem 4.3.2 is now a direct consequence of Proposition 4.3.6 and Proposition 4.3.7.

4.4 Numerical Comparison in Image Segmentation

The aim of this section is to numerically compare our new approximation from Corollary 4.3.3 with the classical Ambrosio-Tortorelli approach. We aim for a simple and easy to implement algorithm in order to illustrate the differences between those two models and justify our theory. As an application for the numerical computations we choose the image segmentation problem already described in the introduction.

Thus, for $\Omega \subset \mathbb{R}^n$ being non-empty, open, bounded and with Lipschitz boundary, we seek to minimize the following functional

$$E(u) = \frac{\alpha}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{\beta}{2}\int_\Omega |u-g|^2 \,\mathrm{d}x + \gamma\mathcal{H}^1(S_u) \quad \text{for } u \in \mathrm{SBV}^2(\Omega)\,,$$

where $g \in L^\infty(\Omega)$ is the original image and $\alpha, \beta, \gamma > 0$ are the parameters influencing the smoothing and segment detection in the solution. They have, of course, to be chosen with care in order to get a sensible result.

Using now Corollary 4.3.3 and the fact that Γ-convergence is stable under continuous perturbations we can approximately minimize E by minimizing

$$\mathcal{B}_\varepsilon(u,v) := \frac{\alpha}{2}\int_\Omega v^2|\nabla u|^2 \,\mathrm{d}x + \frac{\beta}{2}\int_\Omega |u-g|^2 \,\mathrm{d}x + \frac{\gamma}{2\varepsilon}\int_\Omega (1-v)\,\mathrm{d}x + \frac{\gamma}{2}|\mathrm{D}v|(\Omega)\,, \quad (4.36)$$

for small $\varepsilon > 0$, which we also refer to as the BV-*model*.

On the other hand we consider the elliptic approximation, similar to (4.1), which has been introduced in [12] and writes like

$$\mathcal{AT}_\varepsilon(u,v) := \frac{\alpha}{2}\int_\Omega v^2|\nabla u|^2 \,\mathrm{d}x + \frac{\beta}{2}\int_\Omega |u-g|^2 \,\mathrm{d}x \\ + \gamma\int_\Omega \frac{1}{4\epsilon}(1-v)^2 + \varepsilon|\nabla v|^2 \,\mathrm{d}x \quad (4.37)$$

for $u \in H^1(\Omega)$ and $v \in H^1(\Omega;[0,1])$, which we refer to as the H^1-model (note that we “redefined” $\mathcal{AT}_\varepsilon$ as in the following, we will only use (4.37) such that there is no chance of confusion). Further, we chose $\eta_\varepsilon = 0$ as discussed in Remark 4.3.4, which clearly also holds for the Ambrosio-Tortorelli approximation.

For the discretization of these functionals we consider a 2-dimensional image with its natural pixel grid with pixel length $h > 0$. If the picture is given by $M \times N$ pixels, we use the discrete grid $\Omega_h = \{h, \dots, Mh\} \times \{h, \dots Nh\}$ and we identify the functions u, g, v as elements in the Euclidean space $\mathbb{R}^{M\times N}$. Precisely, one sets $u = \sum_{ij} u_{ij}\chi_{[(i-1)h,ih)\times[(j-1)h,jh)}$ for $(u_{ij}) \in \mathbb{R}^{M\times N}$.

For the discretization of the appearing gradients and the total variation we use a finite difference scheme. For this purpose we define the finite difference operator

$$(\nabla_h u)_{ij} = \big((\nabla_h^{(1)}u)_{ij}, (\nabla_h^{(2)}u)_{ij}\big) \quad \text{for } u \in \mathbb{R}^{M\times N}$$

by

$$
\begin{aligned}
(\nabla_h^{(1)} u)_{ij} &:= \frac{u_{i+1,j} - u_{ij}}{h} && \text{for } i \in \{1, \dots, M-1\}, j \in \{1, \dots, N\}, \\
(\nabla_h^{(1)} u)_{Mj} &:= 0 && \text{for } j \in \{1, \dots, N\}, \\
(\nabla_h^{(2)} u)_{ij} &:= \frac{u_{i,j+1} - u_{ij}}{h} && \text{for } i \in \{1, \dots, M\}, j \in \{1, \dots, N-1\}, \\
(\nabla_h^{(2)} u)_{iN} &:= 0 && \text{for } i \in \{1, \dots, M\}.
\end{aligned}
$$

Furthermore we denote the adjoint or transposed of ∇_h by $-\operatorname{div}_h$. For functions $u, v \in \mathbb{R}^{M \times N}$, operations such as the product uv (or $u \cdot v$), the minimum $u \wedge v$, the maximum $u \vee v$, and the square u^2 are always meant to be element-wise. With $\|u\|_2$, $\|u\|_1$ and $\|u\|_\infty$ we respectively refer to the Frobenius norm, the ℓ^1-norm of u vectorized, and the maximum norm of u. The Frobenius inner product of u and v is written as $\langle u, v \rangle$. For any field $q = (q^{(1)}, q^{(2)}) \in \mathbb{R}^{2 \times M \times N}$, like $\nabla_h u$ for $u \in \mathbb{R}^{M \times N}$, we denote by $|q|$ the Euclidean norm along the first axis, i.e. $|q| \in \mathbb{R}^{M \times N}$

$$
|q|_{ij} = \sqrt{\big(q_{ij}^{(1)}\big)^2 + \big(q_{ij}^{(2)}\big)^2}.
$$

With this strategy we can define the discretized versions of (4.36) and (4.37), respectively, for all $u, v \in \mathbb{R}^{M \times N}$ by

$$
\mathcal{B}_\varepsilon^h(u, v) := \frac{\alpha}{2} \big\| v |\nabla_h u| \big\|_2^2 + \frac{\beta}{2} \|u - g\|_2^2 + \frac{\gamma}{2\varepsilon} \langle \mathbb{1}, \mathbb{1} - v \rangle + \frac{\gamma}{2} \big\| |\nabla_h v| \big\|_1 + \chi_{\{0 \le v \le \mathbb{1}\}}(v)
$$

and

$$
\mathcal{AT}_\varepsilon^h(u, v) := \frac{\alpha}{2} \big\| v |\nabla_h u| \big\|_2^2 + \frac{\beta}{2} \|u - g\|_2^2 + \frac{\gamma}{4\varepsilon} \|\mathbb{1} - v\|_2^2 + \gamma\varepsilon \big\| |\nabla_h v| \big\|_2^2 + \chi_{\{0 \le v \le \mathbb{1}\}}(v).
$$

The symbol $\mathbb{1}$ refers to the discretized function that is one almost everywhere. Note that we neglected the factor h^2 in the functionals since it does not change their minimum.

Remark 4.4.1. The choice of the recovery sequence in the proof of Proposition 4.3.7 suggests that $\varepsilon > 0$ represents the width of the detected contours represented by the phase field variable v. Although, we would like to have this parameter extremely small, there is a limit of choice depending on the pixel size h. To be more precise, choosing $h_\varepsilon > 0$ depending on ε, it is well known that $\mathcal{AT}_\varepsilon^{h_\varepsilon}$ Γ-converges as $\varepsilon \to 0$ only for $h_\varepsilon \ll \varepsilon$ (see [22, 28]).

The difficulty in finding the minimizer lies in the non-convex, and for $\mathcal{B}_\varepsilon^h$ also non-smooth, structure. In previous works an alternating minimization scheme has been commonly used, exploiting the fact that the functionals are convex in each variable separately (see [2, 16, 28]). However, in this work we choose a more recent approach, which is the proximal alternating linearized minimization (in short PALM) presented in [24]. This algorithm is a form of an alternating gradient descent procedure, for which we do not have to solve any linear equation. This makes the algorithm also faster than the alternating minimization scheme, especially for rather large images.

For the PALM algorithm one uses the fact that the objective functional can be written as $J(u,v) + G(u) + H(v)$. Then, for some initial value $u^0, v^0 \in \mathbb{R}^{M\times N}$ we set for each $k \in \mathbb{N}$

$$u^k = \operatorname{prox}^G_{t_k}\big(u^{k-1} - t_k \nabla_u J(u^{k-1}, v^{k-1})\big) \tag{4.38}$$

$$v^k = \operatorname{prox}^H_{s_k}\big(v^{k-1} - s_k \nabla_v J(u^k, v^{k-1})\big)\,, \tag{4.39}$$

where $t_k, s_k > 0$. By prox^g_t we denote the proximal operator with step size $t > 0$:

$$\operatorname{prox}^g_t(w) = \operatorname*{arg\,min}_{u\in\mathbb{R}^{M\times N}} \left(\frac{1}{2t}\|u-w\|_2^2 + g(u)\right).$$

For the right choices of the step sizes t_k and s_k above one can show that this scheme converges to a critical point of $J(u,v)+G(u)+H(v)$ as $k\to\infty$ (see [24, Proposition 3.1]). Namely, we need to choose $t_k = \frac{\theta_1}{L_1(v_{k-1})}$ and $s_k = \frac{\theta_2}{L_2(u_k)}$ for some $\theta_1, \theta_2 \in (0,1)$, where $L_1(v)$ and $L_2(u)$ are Lipschitz constants of $u \mapsto \nabla_u J(u,v)$ and $v \mapsto \nabla_v J(u,v)$, respectively. Unfortunately, convergence rates are not known, so that as a stopping criterion we are limited to measure the change of the variables in each iteration. We stop the scheme when this change drops under a specified threshold or if a certain maximum of iteration is reached.

We will now have a closer look how the algorithm looks like for $\mathcal{B}^h_\varepsilon$ and $\mathcal{AT}^h_\varepsilon$ separately.

BV-**model**

We write $\mathcal{B}^h_\varepsilon(u,v) = J(u,v) + G(u) + H(v)$ with

$$J(u,v) = \frac{\alpha}{2}\big\|v|\nabla_h u|\big\|^2\,, \quad G(u) = \frac{\beta}{2}\|u-g\|_2^2 \tag{4.40}$$

and

$$H(v) = \frac{\gamma}{2\varepsilon}\langle \mathbb{1}, \mathbb{1} - v\rangle + \frac{\gamma}{2}\big\||\nabla_h v|\big\|_1 + \chi_{\{0\le v\le 1\}}(v)\,.$$

We have

$$\nabla_u J(u,v) = -\alpha \operatorname{div}_h\big(v^2\nabla_h u\big) \quad \text{and} \quad \nabla_v J(u,v) = \alpha v|\nabla_h u|^2\,.$$

Since there holds $\|\nabla_h\|^2 < \frac{8}{h^2}$ we can choose for some $\theta \in (0,1)$

$$t_k = \frac{h^2}{8\alpha} \quad \text{and} \quad s_k = \frac{\theta}{\alpha\big\||\nabla_h u^k|^2\big\|_\infty}\,, \tag{4.41}$$

such that $t = t_k$ is constant throughout the algorithm.

As a simple computation shows, solving (4.38) is then equivalent to

$$u^k = \frac{\bar u^k + t\beta g}{1+t\beta} \quad \text{with} \quad \bar u^k = u^{k-1} + t\alpha \operatorname{div}_h\big((v^{k-1})^2\nabla_h u^{k-1}\big)\,. \tag{4.42}$$

From (4.39) we get the equivalent problem

$$v^k \in \operatorname*{arg\,min}_{v\in\mathbb{R}^{M\times N}} \Big(\frac{1}{2}\Big\| v - \bar{v}^k - \frac{\gamma s_k}{2\varepsilon}\mathbb{1}\Big\|_2^2 + \frac{\gamma s_k}{2}\big\| |\nabla_h v|\big\|_1 + \chi_{\{0\le v\le \mathbb{1}\}}(v)\Big) \tag{4.43}$$

with $\bar{v}^k = v^{k-1} - s_k \alpha v^{k-1}|\nabla_h u^k|^2$. Since the non-smooth term $\||\nabla_h v|\|_1$ is still present, this minimization can not be solved directly. Instead we tackle it with the algorithm introduced by A. Chambolle and T. Pock in [43], solving the corresponding primal-dual problem. Therefore, we define for all $v \in \mathbb{R}^{M\times N}$ and $w \in \mathbb{R}^{2\times M\times N}$ the functions

$$P_k(v) = \frac{1}{2}\Big\| v - \bar{v}^k - \frac{\gamma s_k}{2\varepsilon}\mathbb{1}\Big\|_2^2 + \chi_{\{0\le v\le 1\}}(v) \quad \text{and} \quad Q_k(w) = \frac{\gamma s_k}{2h}\big\||w|\big\|_1$$

such that (4.43) is equivalent to

$$v^k \in \operatorname{arg\,min}\big\{P_k(v) + Q_k(\nabla_1 v) : v \in \mathbb{R}^{M\times N}\big\}\,. \tag{4.44}$$

The corresponding primal-dual saddle point problem is given by

$$\min_{p\in\mathbb{R}^{M\times N}} \max_{q\in\mathbb{R}^{2\times M\times N}} \big(\langle \nabla_1 p, q\rangle + P_k(p) - Q_k^*(q)\big) \tag{4.45}$$

where Q_k^* denotes the convex conjugate of Q_k, i.e., $Q_k^* = \chi_{\{\|\cdot\|_\infty \le \frac{\gamma s_k}{2h}\}}$. Clearly, for any solution (p, q) of (4.45) we have that $v^k = p$ is a solution of (4.44). We solve (4.45) with [43, Algorithm 1]. Namely, for $0 < \tau^2 \le \frac{1}{8}$ and for some $p_k^0 \in \mathbb{R}^{M\times N}$, $q_k^0 \in \mathbb{R}^{2\times M\times N}$ as well as $\hat{p}_k^0 := p_k^0$ we define for all $\ell \in \mathbb{N}$

$$q_k^\ell = \operatorname{prox}_\tau^{Q_k^*}\big(q_k^{\ell-1} + \tau\nabla_1 \hat{p}_k^{\ell-1}\big)\,, \tag{4.46}$$

$$p_k^\ell = \operatorname{prox}_\tau^{P_k}\big(p_k^{\ell-1} + \tau \operatorname{div}_1 q_k^\ell\big)\,, \tag{4.47}$$

$$\hat{p}_k^\ell = 2p_k^\ell - p_k^{\ell-1}\,. \tag{4.48}$$

Then, [43, Theorem 1] guarantees the convergence of (p_k^ℓ, q_k^ℓ) as $\ell \to \infty$ to a solution of (4.45). For a stopping criterion of the primal-dual iteration we consider the primal-dual gap which is for $p \in \mathbb{R}^{M\times N}$ and $q \in \mathbb{R}^{2\times M\times N}$ given by

$$\mathcal{G}_k(p,q) = P_k(p) + Q_k(\nabla_1 p) + P_k^*(\operatorname{div}_1 q) + Q_k^*(q)\,.$$

It vanishes if and only if (p, q) solves (4.45). For this reason we stop iteration (4.46)–(4.48) if the corresponding primal-dual gap is smaller than a certain tolerance.

We now continue with the precise computations of the primal-dual steps for the BV-phase field approximation. Since Q_k^* is the indicator function of a convex set, the update step (4.46) is the projection of $q_k^{\ell-1} + \tau\nabla_1\hat{p}_k^{\ell-1}$ onto $\{\|\cdot\|_\infty \le \frac{\gamma s_k}{2h}\}$ (cf. [43, Section 6.2]). Thus we simply get

$$q_k^\ell = \frac{\bar{q}_k^\ell}{\mathbb{1} \vee \frac{2h|\bar{q}_k^\ell|}{\gamma s_k}} \quad \text{with} \quad \bar{q}_k^\ell = q_k^{\ell-1} + \tau\nabla_1\hat{p}_k^{\ell-1}\,.$$

The proximal operator appearing in (4.47) can be solved directly. Namely, we get

$$0 \in \frac{1+\tau}{\tau} p_k^\ell - \frac{1}{\tau}\bar{p}_k^\ell - \bar{v}^k - \frac{\gamma s_k}{2\varepsilon}\mathbb{1} + \partial\chi_{\{0\le p\le \mathbb{1}\}}(p_k^\ell)$$

with $\bar{p}_k^\ell = p_k^{\ell-1} + \tau \operatorname{div}_1 q_k^\ell$, which yields

$$p_k^\ell = 0 \vee \left(\frac{\bar{p}_k^\ell + \tau\bar{v}^k + \tau\frac{\gamma s_k}{2\varepsilon}\mathbb{1}}{1+\tau}\right) \wedge \mathbb{1}\,.$$

The primal-dual gap for p_k^ℓ and q_k^ℓ can be computed explicitly and is given by

$$\mathcal{G}_k(p^\ell, q^\ell) = \frac{\gamma s_k}{2h}\big\||\nabla_1 p_k^\ell|\big\|_1 + \langle (p_k^\ell)', \operatorname{div}_1 q_k^\ell\rangle + \frac{1}{2}(\|p_k^\ell\|_2^2 - \|(p_k^\ell)'\|_2^2) - \left\langle p_k^\ell - (p_k^\ell)', \bar{v}^k + \frac{\gamma s_k}{2\varepsilon}\mathbb{1}\right\rangle$$

with

$$(p_k^\ell)' = 0 \vee \left(\bar{v}^k + \frac{\gamma s_k}{2\varepsilon}\mathbb{1} + \operatorname{div}_1 q_k^\ell\right) \wedge 1\,.$$

Summing up all the previous computations for our BV-phase field model, we get Algorithm 4.1 (at the end of this section) as the numerical scheme as we implement it.

H^1-model (Ambrosio-Tortorelli)

For the elliptic approximation we use J and G as in (4.40) and only redefine H by

$$H(v) = \frac{\gamma}{4\varepsilon}\|\mathbb{1} - v\|_2^2 + \gamma\varepsilon\big\||\nabla_h v|\big\|_2^2 + \chi_{\{0\le v\le \mathbb{1}\}}(v)$$

in order to obtain $\mathcal{AT}_\varepsilon^h(u,v) = J(u,v) + G(u) + H(v)$. Clearly, s_k and $t = t_k$ can also be chosen as before in (4.41). Hence, (4.38) results again in (4.42). The difference of the algorithm compared to the one for the BV-phase field appears in (4.39), which is now equivalent to

$$v^k \in \operatorname*{arg\,min}_{v\in\mathbb{R}^{M\times N}}\left(\frac{1}{2}\left\|v - \frac{2\varepsilon\bar{v}^k + \gamma s_k\mathbb{1}}{2\varepsilon + \gamma s_k}\right\|_2^2 + \frac{2\gamma\varepsilon^2 s_k}{2\varepsilon+\gamma s_k}\big\||\nabla_h v|\big\|_2^2 + \chi_{\{0\le v\le \mathbb{1}\}}(v)\right).$$

Since this problem is sufficiently smooth it could be easily solved directly, by solving a linear system. Nevertheless, for a better comparability and for saving the effort of solving a large linear equation, we stay as close as possible to the algorithm for the BV-model. Thus, we use again the primal-dual scheme as in (4.46)–(4.48), where this time we need to choose

$$P_k(v) = \frac{1}{2}\left\|v - \frac{2\varepsilon\bar{v}^k + \gamma s_k\mathbb{1}}{2\varepsilon + \gamma s_k}\right\|_2^2 + \chi_{\{0\le v\le \mathbb{1}\}}(v)$$

Table 4.1: Numerical parameters

α	β	γ	θ	Tol_1	Tol_2	$MaxIt$
$1.75 \cdot 10^{-4}$	1	$3 \cdot 10^{-5}$	0.99	10^{-3}	10^{-5}	10000

for $v \in \mathbb{R}^{M \times N}$ and

$$Q_k(w) = \frac{\mu}{2} \| |w| \|_2^2 \quad \text{with} \quad \mu = \frac{4\gamma\varepsilon^2 s_k}{h^2(2\varepsilon + \gamma s_k)}$$

for $w \in \mathbb{R}^{2 \times M \times N}$. Note, that we have $Q_k^*(w) = \frac{1}{2\mu} \| |w| \|_2^2$ and thus (4.46) yields

$$q_k^\ell = \frac{\mu}{\mu + \tau} \bar{q}_k^\ell \quad \text{with} \quad \bar{q}_k^\ell = q_k^{\ell-1} + \tau \nabla_1 \hat{p}_k^{\ell-1} ,$$

and (4.47) results in

$$p_k^\ell = 0 \vee \left(\frac{1}{1+\tau} \bar{p}_k^\ell + \frac{\tau(2\varepsilon \bar{v}^k + \gamma s_k \mathbb{1})}{(1+\tau)(2\varepsilon + \gamma s_k)} \right) \wedge \mathbb{1} \quad \text{with} \quad \bar{p}_k^\ell = p_k^{\ell-1} + \tau \operatorname{div}_1 q_k^\ell .$$

The primal-dual gap for this approximation is given by

$$\begin{aligned} \mathcal{G}_k(p_k^\ell, q_k^\ell) = \frac{\mu}{2} \| |\nabla_1 p_k^\ell| \|_2^2 + \langle \operatorname{div}_1 q_k^\ell, (p_k^\ell)' \rangle + \frac{1}{2\mu} \| |q_k^\ell| \|_2^2 \\ + \frac{1}{2} (\| p_k^\ell \|_2^2 - \| (p_k^\ell)' \|_2^2) - \left\langle p_k^\ell - (p_k^\ell)', \frac{2\varepsilon \bar{v}^k + \gamma s_k \mathbb{1}}{2\varepsilon + \gamma s_k} \right\rangle \end{aligned}$$

with

$$(p_k^\ell)' = 0 \vee \left(\frac{2\varepsilon \bar{v}^k + \gamma s_k \mathbb{1}}{2\varepsilon + \gamma s_k} + \operatorname{div}_1 q_k \right) \wedge \mathbb{1} .$$

Altogether, this yields Algorithm 4.2 at the end of this section, which is the numerical scheme that we use for computations.

Numerical Results

With the presented algorithms we perform computations for two different images. For all numerical examples we fix the width of the images to 1. The pixel size h then depends on the number of pixels and is given by $h = \frac{L}{\textit{number of horizontal pixels}}$.

For the first computation we use the noisy image from Figure 4.1. The latter is generated by adding Gaussian noise of standard deviation 0.1 and clipping the result to the original image range $[0, 1]$. In this computation, the input image g corresponds to this noisy image and we only change the approximating variable ε, in order to investigate its influence, while fixing the other parameters for the algorithms as indicated in Table 4.1. The result can be observed in Figure 4.2.

One can clearly see that the BV-model produces almost binary phase fields, i.e. v takes only the values 0 (corresponding to a black pixel) and 1 (corresponding to a white

original image[1] noisy image

Figure 4.1: Input image with 256 x 256 pixels for the computations shown in Figure 4.2.

pixel). In other words these phase fields are much sharper than the ones produced by the H^1-model. Moreover, we observe that ε can be chosen larger when using the BV-model in order to obtain a result that is comparable to the H^1-model.

Besides the comparison of the two models one can also observe, that in both approximations of the Mumford-Shah functional, only few edges are detected if ε is too small. Whereas, if ε is relatively large, the contours become rather wide. These effects are well-known and have already been mentioned in Remark 4.4.1, from which we also expect that for small values of ε, the phase field may detect the edges again, when reducing h. Also this can be confirmed from Figure 4.3, where we use the same image but this time with 512×512 pixels keeping the width of the image domain fixed to 1 as above, resulting in the value of h being halved.

Figure 4.4 shows another picture with 512×512 pixel size. To the original image we again add Gaussian noise (noise level: 0.1). This noisy image serves as the input data g for our algorithms. Besides α and γ, the parameters have been chosen like in Table 4.1.

[1]photo credit: Irina Patrascu Gheorghita: alina's eye `https://www.flickr.com/photos/angel_ina/3201337190/` License: CC-BY 2.0 `https://creativecommons.org/licenses/by/2.0/`

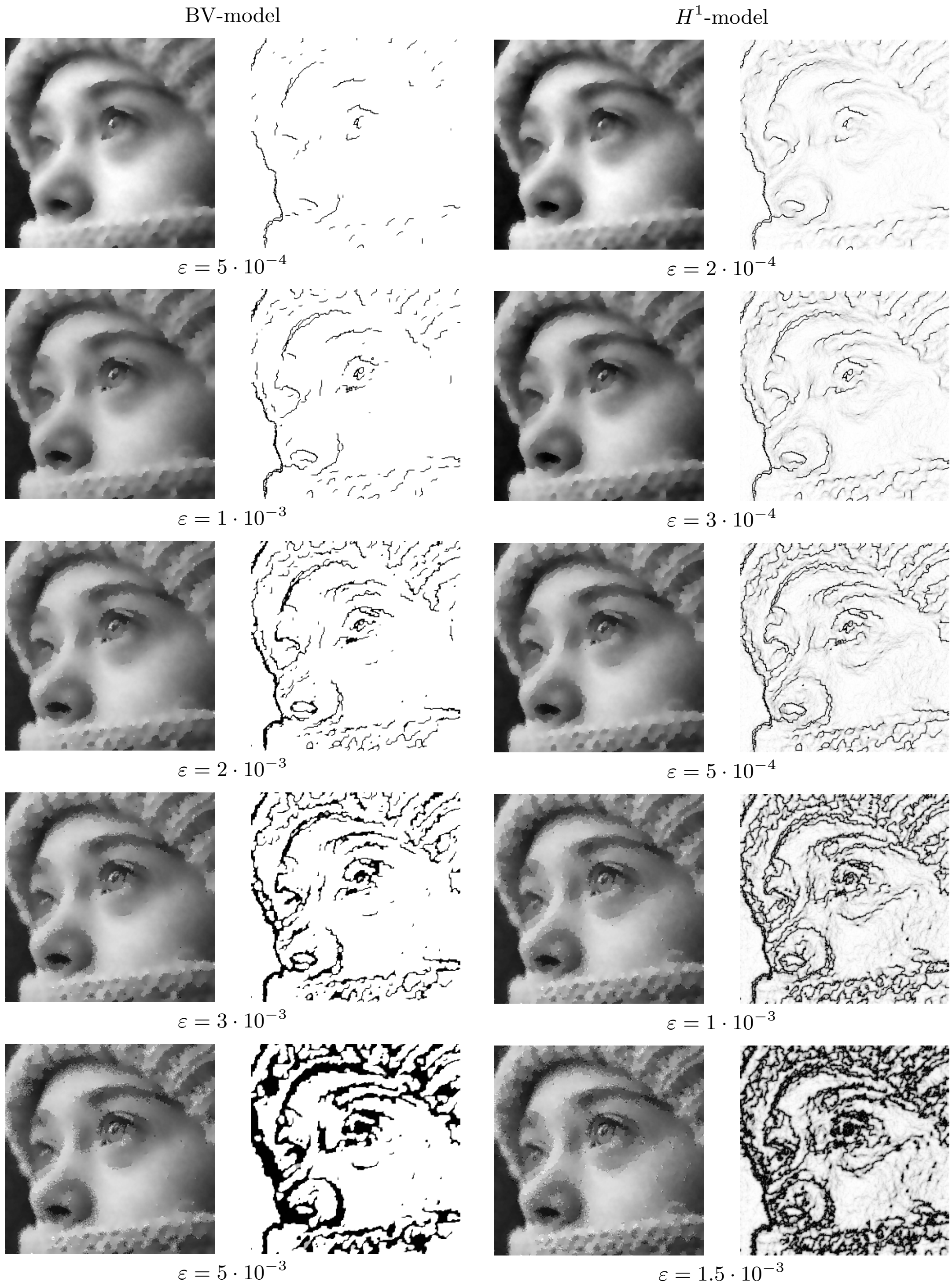
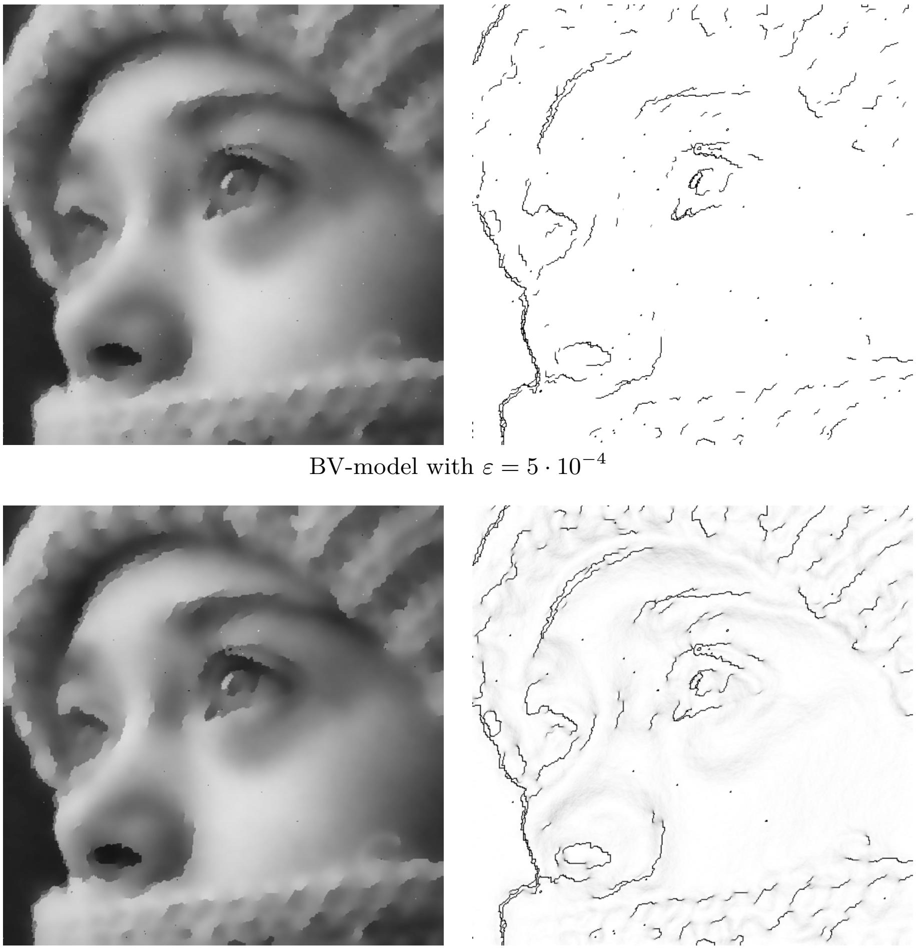


Figure 4.2: Numerical result for different values of ε and for other parameters like in Table 4.1 and different.

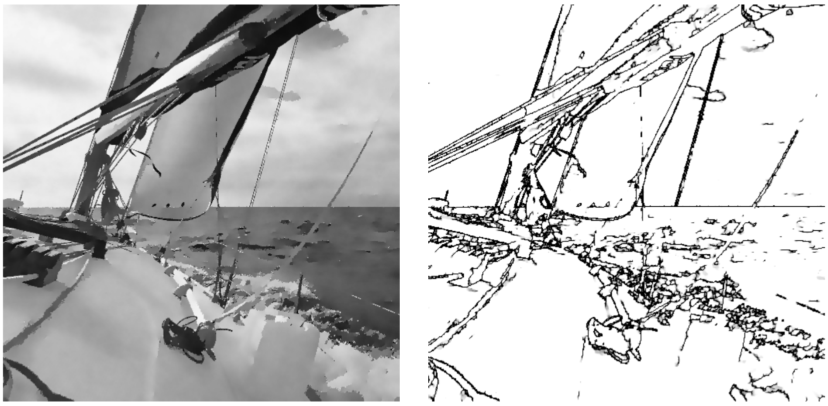


BV-model with $\varepsilon = 5 \cdot 10^{-4}$

H^1-model with $\varepsilon = 2 \cdot 10^{-4}$

Figure 4.3: Result of a segmentally denoised image with 512 x 512 pixels and parameters from Table 4.1.

original image[2] noisy image



BV-model with $\varepsilon = 1 \cdot 10^{-3}$

H^1-model with $\varepsilon = 3 \cdot 10^{-4}$

Figure 4.4: Image with 512 x 512 pixels. Computation for $\alpha = 10^{-4}$, $\gamma = 5 \cdot 10^{-6}$ and the other parameters as specified in Table 4.1.

[2]photo credit: Phuketian.S: *Sailing from Thailand to Malaysia. Our yacht at the sea* `https://www.flickr.com/photos/124790945@N06/32397550408/` License: CC-BY 2.0 `https://creativecommons.org/licenses/by/2.0/`

Algorithm 4.1 BV-model

$u \leftarrow g,\ v \leftarrow 1,\ q \leftarrow 0$

$t \leftarrow \dfrac{h^2}{8\alpha},\ \tau \leftarrow \dfrac{1}{\sqrt{8}}$

$it \leftarrow 0$

repeat

  $it \leftarrow it + 1$

  $u_0 \leftarrow u,\ v_0 \leftarrow v$

  $u \leftarrow \dfrac{u + t\alpha\,\mathrm{div}_h(v^2 \nabla_h u) + t\beta g}{1 + t\beta}$

  $s \leftarrow \dfrac{\theta}{\alpha \| |\nabla_h u|^2 \|_\infty}$

  $p \leftarrow v,\ \hat{p} \leftarrow v$

  $\bar{v} \leftarrow v - s\alpha v |\nabla_h u|^2$

  repeat

    $p_0 \leftarrow p$

    $\bar{q} \leftarrow q + \tau \nabla_1 \hat{p}$

    $q \leftarrow \dfrac{\bar{q}}{1 \vee \frac{2h}{\gamma s} |\bar{q}|}$

    $\bar{p} \leftarrow p + \tau\, \mathrm{div}_1\, q$

    $p \leftarrow 0 \vee \left(\dfrac{\bar{p} + \tau \bar{v} + \frac{\gamma \tau s}{2\varepsilon} \mathbb{1}}{1 + \tau} \right) \wedge \mathbb{1}$

    $p' \leftarrow 0 \vee \left(\bar{v} + \dfrac{\gamma s}{2\varepsilon} \mathbb{1} + \mathrm{div}_1\, q \right) \wedge \mathbb{1}$

    $\hat{p} \leftarrow 2p - p_0$

    $gap \leftarrow \dfrac{1}{2} \left(\|p\|_2^2 - \|p'\|_2^2 \right) - \left\langle p - p', \bar{v} + \dfrac{\gamma s}{2\varepsilon} \mathbb{1} \right\rangle$

  until $gap + \dfrac{\gamma s}{2h} \big\| |\nabla_1 p| \big\|_1 + \langle \mathrm{div}_1\, q, p' \rangle \leq Tol_2$

  $v \leftarrow p$

until $\max\{ \|v - v_0\|_\infty, \|u - u_0\|_\infty \} \leq Tol_1$ **or** $it = MaxIt$

Algorithm 4.2 H^1-model

$u \leftarrow g$, $v \leftarrow 1$, $q \leftarrow 0$

$t \leftarrow \frac{h^2}{8\alpha}$, $\tau \leftarrow \frac{1}{\sqrt{8}}$

$it \leftarrow 0$

repeat

  $it \leftarrow it + 1$

  $u_0 \leftarrow u$, $v_0 \leftarrow v$

  $u \leftarrow \frac{u + t\alpha \operatorname{div}_h(v^2 \nabla_h u) + t\beta g}{1 + t\beta}$

  $s \leftarrow \frac{\theta}{\alpha \| |\nabla_h u|^2 \|_\infty}$

  $p \leftarrow v$, $\hat{p} \leftarrow v$

  $\bar{v} \leftarrow v - s\alpha v |\nabla_h u|^2$

  $\mu \leftarrow \frac{4\gamma\varepsilon^2 s}{h^2(2\varepsilon + \gamma s)}$

  repeat

    $p_0 \leftarrow p$

    $\bar{q} \leftarrow q + \tau \nabla_1 \hat{p}$

    $q \leftarrow \frac{\mu}{\mu + \tau} \bar{q}$

    $p \leftarrow 0 \vee \left(\frac{1}{1+\tau} \bar{p} + \frac{\tau(2\varepsilon\bar{v} + \gamma s \mathbb{1})}{(1+\tau)(2\varepsilon + \gamma s)} \right) \wedge \mathbb{1}$

    $p' \leftarrow 0 \vee \left(\frac{2\varepsilon\bar{v} + \gamma s \mathbb{1}}{2\varepsilon + \gamma s} + \operatorname{div}_1 q \right) \wedge \mathbb{1}$

    $\hat{p} \leftarrow 2p - p_0$

    $gap \leftarrow \frac{1}{2}(\|p\|_2^2 - \|p'\|_2^2) - \left\langle p - p', \frac{2\varepsilon\bar{v} + \gamma s \mathbb{1}}{2\varepsilon s + \gamma s} \right\rangle$

  until $gap + \frac{\mu}{2} \| |\nabla_1 p| \|_2^2 + \langle \operatorname{div}_1 q, p' \rangle + \frac{1}{2\mu} \| |q| \|_2^2 \leq Tol_2$

  $v \leftarrow p$

until $\max\{\|v - v_0\|_\infty, \|u - u_0\|_\infty\} \leq Tol_1$ **or** $it = MaxIt$

5 Time Evolutions of an Alternating Minimization Scheme

Phase field models as we have seen them in the previous chapter has gained popularity for numerical computations of minimizers of the Mumford-Shah functional since 1999, when B. Bourdin computed some segmental image denoising in [28]. Simulations for fracture mechanics followed in [15, 16, 17, 26, 27, 29, 38, 39, 40]. All the sources have in common that they use an alternating minimization scheme, exploiting the fact that the phase field models are convex in each variable separately.

In this chapter we study time evolutions obtained from such alternating schemes, but with new implementation of the irreversibility condition inspired from [102]. Moreover, we focus on phase field models of the following form:

$$\mathcal{F}_\varepsilon(u,v) := \frac{1}{2}\int_\omega b|u|^2\,\mathrm{d}x + \int_\omega (v^2+\eta_\varepsilon)\nabla u^\top A_1 \nabla u\,\mathrm{d}x + \\ \kappa\int_\omega \frac{1}{4\varepsilon}(1-v)^2 K + \varepsilon\,\nabla v^\top A_2 \nabla v\,\mathrm{d}x\,, \quad (5.1)$$

where A_1, A_2 are symmetric matrix functions that are uniformly positive definite and K, b are real functions. This setting covers the phase field approximation for the fracture models of thin elastic shells, that we derived in (4.25). It is recovered for $A_1 = A_2 = (a^{\alpha\beta})\sqrt{a}$, $K = \sqrt{a}$ and $b = \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma,\tau}\sqrt{a}$.

The content of this chapter of the thesis is extracted from the publication [1]. It was developed together with M. Negri and S. Almi and deals with the classical Ambrosio-Tortorelli functional. Here, we present an adaption of the cited material to (5.1).

For technical reasons, we stick from now on to the dimension $n = 2$, i.e. we assume that $\omega \subset \mathbb{R}^2$. For the time evolution let us consider a time interval $[0,T]$ (for some $T > 0$) and a a function $g(t)$ for each $t \in [0,T]$ describing the time dependent boundary condition on $\partial\omega$ for u. Furthermore, we suppose to have some initial conditions u_0 and v_0. As usual in the theory of rate-independent processes (see e.g. [94, 95]) we use a time discretization as follows: For every $k \in \mathbb{N}$ we set the time step size $\tau_k := \frac{T}{k}$, and we consider the time steps $t_i^k := i\tau_k$ for $i \in \{0,\ldots,k\}$.

The standard alternating minimization scheme would now be the following:

$$u_{i,j}^k := \arg\min\{\mathcal{F}_\varepsilon(u, v_{i,j-1}^k) : u \in H^1(\omega), u = g(t_i^k) \text{ on } \partial\omega\}\,, \quad (5.2)$$

$$v_{i,j}^k := \arg\min\{\mathcal{F}_\varepsilon(u_{i,j}^k, v) : v \in H^1(\omega), v \le v_{i,j-1}^k\}\,. \quad (5.3)$$

It can be easily seen that this scheme converges for $j \to \infty$ to a critical point of $\mathcal{F}_\varepsilon$ (see e.g. [39, Proposition 2]). For this reason one sets

$$u_i^k := \lim_{j\to+\infty} u_{i,j}^k \qquad \text{and} \qquad v_i^k := \lim_{j\to+\infty} v_{i,j}^k\,.$$

For $\mathcal{F}_\varepsilon$ being the classical Ambrosio-Tortorelli functional from (1.6) the limits for $k \to \infty$, or equivalently for $\tau_k \to 0$, of these discrete evolutions has been investigated in [87]. In some sense the obtained time-continuous evolutions provide an approximation of a quasi-static evolution for brittle fracture. In [2] we studied a space discrete version of this alternating scheme and showed its consistency in the sense that the space discrete time evolution converge to the space continuous one as the mesh size tends to zero.

Let us now have a look on the inequality constraint, $v \le v_{i,j-1}^k$, in the minimization (5.3) with respect to the phase field variable, which represents the irreversibility condition. In the literature one can find also other approaches for imposing the irreversibility condition. For instance the inequality constrained is sometimes replaced by a sublevel approach, setting v equal to zero where it becomes smaller than a certain threshold (see e.g. [15, 27, 38]). This is mainly done for a better efficiency in the numerical computations but lacks, as far as we know, a rigorous theoretical treatment.

As already indicated at the beginning of this chapter we follow another approach here that comes from [102], using a pointwise minimization instead of an inequality constrained. This is computationally very convenient and still physically correct. With the notation used above and with u_{i-1}^k, v_{i-1}^k (at time t_{i-1}^k) already known we precisely set for all $i \in \mathbb{N}$

$$u_i^k := \arg\min\{\mathcal{F}_\varepsilon(u, v_{i,j-1}^k) : u \in H^1(\omega), u = g(t_i^k) \text{ on } \partial\omega\}\,, \tag{5.4}$$

$$\tilde{v}_i^k := \arg\min\left\{\mathcal{F}_\varepsilon(u_i^k, v) + \frac{1}{2\tau_k}\|v - v_{i-1}^k\|_{L^2(\omega)}^2 : v \in H^1(\omega)\right\}, \tag{5.5}$$

$$v_i^k := \min\{\tilde{v}_i^k, v_{i-1}^k\}\,. \tag{5.6}$$

We remark that the monotonicity of v_i^k is taken into account by a simple truncation after an unconstrained minimization. This is numerically more efficient than taking care of an inequality constraint. Further, we presented here the most simple setting by performing only one iteration of the alternating scheme and we added a L^2-distance as a penalization in (5.5). This is actually the setting in [102], and the L^2-penalization is responsible for getting in the limit as $\tau_k \to 0$ a unilateral L^2-gradient flow with respect to the phase field variable. To be more precise, we prove in Section 5.3 that in the limit we obtain an evolution $t \mapsto (u(t), v(t))$ such that

$$u(t) \in \arg\min\{\mathcal{F}_\varepsilon(u, v(t)) : u \in H^1(\omega) \text{ with } u = g(t) \text{ on } \partial\omega\} \quad \text{for all } t \in [0,T]\,,$$

and $0 \le v(t) \le v(s) \le 1$ for all $0 \le t \le s \le T$. Moreover, the following energy balance identity holds:

$$\dot{\mathcal{F}}_\varepsilon(u(t), v(t)) = -\frac{1}{2}\|\dot{v}(t)\|_{L^2}^2 - \frac{1}{2}\left|\partial_v^- \mathcal{F}_\varepsilon\right|^2(u(t), v(t)) + \mathcal{P}(u(t), v(t), \dot{g}(t))\,,$$

where $|\partial_v^- \mathcal{F}_\varepsilon|$ is the L^2-unilateral slope with respect to v, $\mathcal{P}$ is the power of external forces, and the dot denotes the time derivative (for details see Definition 5.1.1 and Proposition 5.1.3). This energy balance is precisely the L^2-gradient flow of v in a weak sense (see [11]). Unilateral L^2-evolutions of this type are frequently employed in computational fracture, in this form and under the name of Ginzburg-Landau models (see, e.g., [5] and the references therein). A system of this type has been studied in [21] and employed, as a regularization, also in [88]. We recall that the vanishing viscosity limit of these rate independent evolutions are indeed quasi-static evolutions in the sense of [88, 98]. A different approach for a unilateral rate-independent model, coupled with elasto-dynamic, can be found in [89].

Similar to the consistency of the space discretization by finite element methods of quasi-static evolutions, which we have shown in [2], we consider in Section 5.4 a space discrete approximation of the unilateral L^2-gradient flow obtained by (5.4)–(5.6). We consider a family of P_1 finite element spaces on acute angle triangulations $\mathcal{T}_h$, i.e.,

$$\begin{aligned} u &\in \{z \in H^1(\omega) : z \text{ is piecewise affine on } \mathcal{T}_h\} \\ v &\in \{z \in H^1(\omega) : z \text{ is piecewise affine on } \mathcal{T}_h\}, \end{aligned}$$

and a family of approximating energies of the form

$$\mathcal{F}_{\varepsilon,h}(u,v) := \frac{1}{2}\int_\omega (\Pi_h(v^2) + \eta_\varepsilon)\nabla u^\top A_1 \nabla u \,\mathrm{d}x \\ + \kappa \int_\omega \frac{1}{4\varepsilon}\Pi_h((1-v)^2)h + \varepsilon\, \nabla v^\top A_2 \nabla v \,\mathrm{d}x\,,$$

where Π_h is the usual Lagrange interpolation operator. We remark that $\mathcal{F}_{\varepsilon,h}$ is not, strictly speaking, the restriction of $\mathcal{F}_\varepsilon$ to the finite element spaces. Nevertheless, it is not too difficult to show that the Γ-limit as $\varepsilon \to 0$ and with $h = o(\varepsilon)$ is again of the form (4.24). Moreover, the operator Π_h and the acute angle triangulations allow to prove that the phase field variable in the space discrete setting takes values in the interval $[0, 1]$ (see [2]).

In this framework, we consider again a time discrete approach in which the incremental problem is obtained by an alternate minimization procedure. This time, however, we imitate (5.2)–(5.3) and repeat (5.4)–(5.6) for each time step multiple times. In this way we hope in view of [38, Proposition 2], to get closer to an equilibrium point. Indeed, we realized that computationally the one step scheme does not provide very good solutions (at least for reasonable time step sizes). As expected in numerical practise one can only perform finitely many iterations, according to some stopping criterion. In order to have a general result, including all possible criteria, we only assume that the number of iterations J_i^k, possibly depending on k and i, are uniformly bounded from above, with respect to k and i, by a certain arbitrarily large number J. Thus, for $i \in \mathbb{N}$, knowing u_{i-1}^k and v_{i-1}^k (at time t_{i-1}^k), we consider the sequences $u_{i,j}^k$ and $v_{i,j}^k$, for $j \in \mathbb{N}$, defined by the following alternating minimization scheme: $u_{i,0}^k := u_{i-1}^k$, $v_{i,0}^k := v_{i-1}^k$, and, for $j = 1, ..., J_i^k$,

$$u_{i,j}^k := \arg\min\{\mathcal{F}_{\varepsilon,h}(u, v_{i,j-1}^k) : u = g(t_i^k) \text{ on } \partial\omega\}\,, \tag{5.7}$$
$$\tilde{v}_{i,j}^k := \arg\min\{\mathcal{F}_{\varepsilon,h}(u_{i,j}^k, v) + \tfrac{1}{2\tau_k}\|v - v_{i-1}^k\|_{L^2}^2\}\,, \tag{5.8}$$
$$v_{i,j}^k := \min\{\tilde{v}_{i,j}^k, v_{i-1}^k\}\,. \tag{5.9}$$

Then set

$$u_i^k := u_{i,J_i^k}^k \qquad \text{and} \qquad v_i^k := v_{i,J_i^k}^k\,.$$

We prove in Theorem 5.4.14 and Theorem 5.4.18 that the limit as $\tau_k \to 0$ and $h \to 0$ is again a unilateral L^2-gradient flow. Note that in the L^2-penalization term and the pointwise minimization, the function v_{i-1}^k, representing the configuration at time t_{i-1}^k, appears and not $v_{i,j-1}^k$, as in the configuration of the alternate scheme (5.2)–(5.3). The sequence $\{v_{i,j}^k\}_{j\in\mathbb{N}}$ may therefore not be monotone, but still satisfies the constraint $v_{i,j}^k \le v_{i-1}^k$ for every j. This choice is again motivated by applications and simulations. Indeed, using $v_{i,j-1}^k$, as in [87], may lead in some cases to accumulation of numerical errors at each iteration.

Finally, in Section 5.5 we provide a detailed set of numerical examples. Our aim is to show and compare the efficiency of the one-step and multi step schemes. For simplicity we conduct these tests a flat domain, thus in an anti-plain strain setting. Computations of the here introduced scheme on curved surfaces follow in Chapter 6. As we have mentioned above, it turns out that the multi-step algorithm is more stable and computationally more convenient than the single-step scheme. In particular, we will see that comparable evolutions are obtained for time step sizes of the order 10^{-1}, using the former algorithm, and for time step sizes of the order 10^{-3}, using the latter. For this reason, the multi-step scheme is computationally faster. We remark again that, from a numerical viewpoint, the power of the alternate minimization scheme investigated in this work lacks an a priori constraints in the phase field minimizations (5.8). In this way, indeed, we are simply led to solve a linear system.

From the technical point of view it is important to stress that our result employs an argument based on a fine regularity estimate, proved in [79] and already employed in [88], together with Sobolev embeddings (see proof of Proposition 5.1.9) which holds only for $\omega \subset \mathbb{R}^2$ and not for higher dimensions. Second, the structure of discrete scheme, with unconstrained minimization and a posteriori truncation makes it very difficult, if not impossible, to obtain H^1 estimates and apply Gronwall type arguments for the speed of the phase field variable. We are thus forced to work only with L^2 velocities and the energy identity cannot rely on the chain rule. We use instead, for the energy identity, the Riemann sum argument of [55].

5.1 Description and Setting of the Problem

Let ω be an open bounded subset of $\mathbb{R}^2$ with Lipschitz boundary $\partial\omega$. Furthermore, let $f \in C^1(\omega)$ be a non-negative, bounded function, and let $A_1, A_2 \colon \omega \to \mathbb{R}^{2\times 2}$ be continuous, such that $A_i(x)$ is a symmetric, positive definite matrix for all $x \in \omega$, $i \in \{1,2\}$. In addition we assume that for each $i \in \{1,2\}$ there exists $c, C > 0$ such that

$$c|\zeta| \leq \zeta^\top A_i(x)\zeta \leq C|\zeta| \quad \text{for all } \zeta \in \mathbb{R}^2, x \in \omega\,. \tag{5.10}$$

For every $u \in H^1(\omega)$ and $v \in H^1(\omega;[0,1])$, we define the *elastic energy*

$$\mathcal{E}(u,v) := \frac{1}{2}\int_\omega b|u|^2 \,\mathrm{d}x + \frac{1}{2}\int_\omega (v^2+\eta)\nabla u^\top A_1 \nabla u \,\mathrm{d}x\,, \tag{5.11}$$

where η is a positive parameter. We remark that, since v and f are bounded and A_1 fulfills (5.10) there holds for some $C > 0$ (only depending on f, A_1 and η)

$$c\|u\|^2_{H^1(\omega)} \leq \mathcal{E}(u,v) \leq C\|u\|^2_{H^1(\omega)} \quad \text{for all } u \in H^1(\omega), v \in H^1(\omega;[0,1])\,. \tag{5.12}$$

We introduce the *dissipation potential* associated to the phase field variable $v \in H^1(\omega;[0,1])$ given by

$$\mathcal{D}(v) := \frac{1}{2}\int_\omega \nabla v^\top A_2 \nabla v + (1-v)^2 h \,\mathrm{d}x\,, \tag{5.13}$$

where $A_2 \colon \omega \to \mathbb{R}^{2\times 2}$ is continuous with $A_2(x)$ being a symmetric, positive definite matrix for all $x \in \omega$. Note that the *dissipation* (i.e., rate of dissipated energy) turns out to be of the form $d\mathcal{D}(v)[\dot{v}]$ (under suitable time regularity of v), where the dot denotes the time derivative.

The *total energy* $\mathcal{F} \colon H^1(\omega) \times H^1(\omega;[0,1]) \to [0,+\infty)$ of the system is given by the sum of elastic energy (5.11) and dissipation potential (5.13), i.e.,

$$\mathcal{F}(u,v) := \mathcal{E}(u,v) + \mathcal{D}(v)\,. \tag{5.14}$$

We notice that the functional $\mathcal{F}$ in (5.14) coincides with $\mathcal{F}_\varepsilon$ in (5.1) for $\varepsilon = \frac{1}{2}$ and $\kappa = 1$. This choice is made for notational convenience and does not influence our analysis.

An important role in the definition of evolution is played by the following notion of *unilateral L^2-slope*.

Definition 5.1.1. For $u \in H^1(\omega)$ and $v \in H^1(\omega;[0,1])$ we define the *unilateral L^2-slope* of $\mathcal{F}$ with respect to v at the point (u,v) as

$$|\partial_v^- \mathcal{F}|(u,v) := \limsup_{\substack{z \to v \\ z \in H^1(\omega;[0,1]),\, z \leq v}} \frac{[\mathcal{F}(u,v) - \mathcal{F}(u,z)]_+}{\|v-z\|_{L^2}}\,, \tag{5.15}$$

where $[\cdot]_+$ denotes the positive part and the convergence is intended in the L^2-topology.

Remark 5.1.2. The minus sign appearing in the notation $|\partial_v^- \mathcal{F}|$ reminds that only negative variations are allowed; it should not be confused with a similar notation for the relaxed slope (see, e.g., [11, Section 2.3]).

For $u \in H^1(\omega)$ and $v, \varphi \in H^1(\omega; [0,1])$ there exists the partial derivative of $\mathcal{F}$ with respect to v, i.e.,

$$\partial_v \mathcal{F}(u,v)[\varphi] = \int_\omega v\varphi \nabla u^\top A_1 \nabla u \,\mathrm{d}x + \int_\omega \nabla v^\top A_2 \nabla\varphi - (1-v)\varphi h \,\mathrm{d}x \,. \tag{5.16}$$

The natural relationship between partial derivatives (5.16) and slope (5.15) is stated in the next lemma.

Lemma 5.1.3. *For $u \in H^1(\omega)$ and $v \in H^1(\omega; [0,1])$ there holds*

$$|\partial_v^- \mathcal{F}|(u,v) = \sup\left\{-\partial_v \mathcal{F}(u,v)[\varphi] : \varphi \in H^1(\omega;[0,1]),\ \varphi \le 0,\ \|\varphi\|_{L^2} \le 1\right\}.$$

Proof. For all $\varphi \in H^1(\omega; [0,1])$ with $\varphi \le 0$ and $\|\varphi\|_{L^2} \le 1$ there holds

$$\begin{aligned}
-\partial_v \mathcal{F}(u,v)[\varphi] &= \lim_{s\to 0^+} \frac{\mathcal{F}(u,v) - \mathcal{F}(u, v+s\varphi)}{s} \\
&\le \limsup_{s\to 0^+} \frac{[\mathcal{F}(u,v) - \mathcal{F}(u,v+s\varphi)]_+}{\|v-(v+s\varphi)\|_{L^2}} \\
&\le \limsup_{\substack{z\to v \\ z\in H^1(\omega;[0,1]), z\le v}} \frac{[\mathcal{F}(u,v)-\mathcal{F}(u,z)]_+}{\|v-z\|_{L^2}} \,.
\end{aligned}$$

Taking the supremum of all φ we get

$$\sup\left\{-\partial_v \mathcal{F}(u,v)[\varphi] : \varphi \in H^1(\omega;[0,1]),\ \varphi \le 0,\ \|\varphi\|_{L^2} \le 1\right\} \le |\partial_v^- \mathcal{F}|(u,v)\,.$$

In order to show the opposite inequality, let (z_n) in $H^1(\omega;[0,1])$ with $z_n \to v$ and $z_n \le v$ for all $n \in \mathbb{N}$ such that

$$\lim_{n\to\infty} \frac{[\mathcal{F}(u,v) - \mathcal{F}(u,z_n)]_+}{\|v-z_n\|_{L^2}} = |\partial_v^- \mathcal{F}|(u,v)\,.$$

We can assume that $|\partial_v^- \mathcal{F}|(u,v) > 0$, otherwise the inequality is obvious since $\partial_v \mathcal{F}(u,v)[0] = 0$. Hence, for n sufficiently large we have $\mathcal{F}(u,v) \ge \mathcal{F}(u,z_n)$. Together with the convexity of $\mathcal{F}(u,\cdot)$ there holds

$$|\partial_v^- \mathcal{F}|(u,v) = \lim_{n\to\infty} \frac{\mathcal{F}(u,v) - \mathcal{F}(u,z_n)}{\|v-z_n\|_{L^2}} \le -\liminf_{n\to\infty} \partial_v \mathcal{F}(u,v)[z_n'],$$

where $z_n' = (z_n - v)/\|v-z_n\|_{L^2}$. Clearly $z_n' \in H^1(\omega;[0,1])$, $z_n' \le 0$ and $\|z_n'\|_{L^2} \le 1$. This concludes the proof of the lemma. □

Finally, let us define, for $u, z \in H^1(\omega)$ and $v \in H^1(\omega;[0,1])$, the functional

$$\mathcal{P}(u,v,z) := \int_\omega buz \,\mathrm{d}x + \int_\omega (v^2+\eta)\nabla u^\top A_1 \nabla z \,\mathrm{d}x \tag{5.17}$$

We anticipate here a continuity property of $\mathcal{P}$ which will be useful in the forthcoming discussion.

Lemma 5.1.4. *If $u_m \rightharpoonup u$ in $H^1(\omega)$ and $v_m \to v$ in $L^2(\omega;[0,1])$, then*

$$\lim_{m\to\infty} \mathcal{P}(u_m, v_m, z) = \mathcal{P}(u, v, z) \quad \textit{for all } z \in H^1(\omega)\,.$$

Proof. Consider a subsequence (not relabelled) such that $v_m \to v$ a.e. in ω. By dominated convergence it is easy to see that $v_m^2 A_1 \nabla z \to v^2 A_1 \nabla z$ strongly in $L^2(\omega;\mathbb{R}^2)$. Thus, with the weak convergence of (u_m), there holds $\mathcal{P}(u_m, v_m, z) \to \mathcal{P}(u, v, z)$. Since this limit is independent of the subsequence, the convergence holds for the whole sequence. □

We are now in a position to give the precise definition of gradient flow evolution we consider in this paper.

Definition 5.1.5. Let $T > 0$ and $g \in AC([0,T]; W^{1,p}(\omega))$ for some $p > 2$. Let $u_0 \in H^1(\omega)$ with $u_0 = g(0)$ on $\partial\omega$ and let $v_0 \in H^1(\omega;[0,1])$ be such that

$$u_0 \in \arg\min\{\mathcal{E}(u, v_0) : u \in H^1(\omega) \text{ with } u = g(0) \text{ on } \partial\omega\}\,.$$

We say that a pair $(u,v)\colon [0,T] \to H^1(\omega) \times H^1(\omega;[0,1])$ is a *unilateral L^2-gradient flow* for the energy $\mathcal{F}$ with initial condition (u_0, v_0) and boundary condition g if the following properties are satisfied:

(a) *Time regularity*: $u \in C([0,T]; H^1(\omega))$ and $v \in H^1([0,T]; L^2(\omega)) \cap L^\infty([0,T]; H^1(\omega))$ with $u(0) = u_0$ and $v(0) = v_0$;

(b) *Irreversibility*: $t \mapsto v(t)$ is non-increasing (i.e., $v(s) \le v(t)$ a.e. in ω for every $0 \le t \le s \le T$) and $0 \le v(t) \le 1$ for every $t \in [0,T]$;

(c) *Displacement equilibrium*: for every $t \in [0,T]$ we have $u(t) = g(t)$ on $\partial\omega$ and

$$u(t) \in \arg\min\left\{\mathcal{E}(u, v(t)) : u \in H^1(\omega) \text{ with } u = g(t) \text{ on } \partial\omega\right\};$$

(d) *Energy balance*: the map $t \mapsto \mathcal{F}(u(t), v(t))$ is absolutely continuous and for a.e. $t \in [0,T]$ it holds

$$\dot{\mathcal{F}}(u(t), v(t)) = -\frac{1}{2}\|\dot{v}(t)\|_{L^2}^2 - \frac{1}{2}|\partial_v^- \mathcal{F}|^2(u(t), v(t)) + \mathcal{P}(u(t), v(t), \dot{g}(t))\,.$$

Remark 5.1.6. Note that $\mathcal{P}(u(t), v(t), \dot{g}(t))$ provides the power of external forces. Indeed, by equilibrium of $u(t)$,

$$\begin{aligned}
\mathcal{P}(u(t), v(t), \dot{g}(t)) &= \int_\omega b u(t)\dot{g}(t)\,\mathrm{d}x - \int_\omega \operatorname{div}\Big((v^2(t)+\eta)A_1\nabla u(t)\Big)\dot{g}(t)\,\mathrm{d}x \\
&\quad + \Big\langle (v^2(t)+\eta)(A_1\nabla u(t))\nu, \dot{g}(t)\Big\rangle_{H^{-\frac{1}{2}}} \\
&= \int_\omega b u(t)\dot{g}(t)\,\mathrm{d}x - \Big\langle (v^2(t)+\eta)(A_1\nabla u(t))\nu, \dot{g}(t)\Big\rangle_{H^{-\frac{1}{2}}}\,,
\end{aligned}$$

where $\langle \cdot, \cdot \rangle$ denotes the duality between $H^{-1/2}(\partial\omega)$ and $H^{1/2}(\partial\omega)$, and ν stands for the exterior unit normal vector to $\partial\omega$. Hence $\mathcal{P}(u(t), v(t), \dot{g}(t))$ gives a weak formulation for the "classic power"

$$\int_\omega bu(t)\dot{g}(t)\,\mathrm{d}x + \int_{\partial\omega} (A_1 \nabla u(t))\nu \dot{g}(t)\,\mathrm{d}\mathcal{H}^1 \,.$$

Remark 5.1.7. If (u, v) is a unilateral L^2-gradient flow in the sense of Definition 5.1.5, one can show that $v \in C([0,T]; H^1(\omega))$. Indeed, if $t_n \to t$ then $u(t_n) \to u(t)$ (strongly) in $H^1(\omega)$ while $v(t_n) \rightharpoonup v(t)$ (weakly) in $H^1(\omega)$. It is not difficult to check that, by the displacement equilibrium (c), $\mathcal{E}(u(t_n), v(t_n)) \to \mathcal{E}(u(t), v(t))$. Hence, the energy balance (d) implies $\mathcal{D}(v(t_n)) \to \mathcal{D}(v(t))$, and, since $v \in C([0,T]; L^2(\omega))$, it follows that

$$\int_\omega |\nabla v(t_n)|^2\,\mathrm{d}x \to \int_\omega |\nabla v(t)|^2\,\mathrm{d}x \,.$$

From this we deduce, together with weak convergence, the continuity of $t \mapsto v(t)$ in $H^1(\omega)$.

Our first goal is to prove the convergence to a unilateral L^2-gradient flow of the *time discrete* solutions obtained by a couple of iterative schemes (see Sections 5.3 and 5.4.2) based on the "unconstrained" version from [102] of the alternate minimization algorithm [27]. Our second aim is to show, in the spirit of [2], that the same convergence result holds true for the corresponding *space and time discrete* scheme, i.e., when also a space discretization is considered, inspired by finite element approximation. We refer to Section 5.4 for the detailed presentation of this last topic.

Before starting any discussion about the construction and convergence of a unilateral L^2-gradient flow, let us comment on the energy equality (d) from Definition 5.1.5. In particular, we show in Proposition 5.1.9 that only an energy inequality is sufficient. The proof is based on a combination of a quantitative regularity estimate proved in [79, Theorem 1.1] and a Riemann sum argument inspired by [55].

Next lemma provides the regularity property needed in our setting. For a more general statement we refer to [79].

Lemma 5.1.8. *Let $g \in AC([0,T]; W^{1,p}(\omega))$ for $p > 2$. For $t \in [0,T]$ and $v \in H^1(\omega; [0,1])$ denote*

$$u(t, v) := \arg\min \{\mathcal{E}(u, v) : u \in H^1(\omega) \text{ with } u = g(t) \text{ on } \partial\omega\} \,.$$

Then there exist an exponent $2 < r < p$ and a constant $C > 0$ such that for every $t_1, t_2 \in [0,T]$ and every $v_1, v_2 \in H^1(\omega; [0,1])$ it holds

$$\|u(t_2, v_2) - u(t_1, v_1)\|_{W^{1,r}} \le C\Big(\|g(t_2) - g(t_1)\|_{W^{1,r}} + \|g\|_{L^\infty(0,T;W^{1,p})}\, \|v_2 - v_1\|_{L^q}\Big) \,,$$

where $1/q = 1/r - 1/p$.

Next proposition shows that the energy inequality (5.18) is actually equivalent to the energy identity (d) of Definition 5.1.5.

Proposition 5.1.9. *Let T, g, u_0 and v_0 be as in Definition 5.1.5. Assume that the pair $(u,v)\colon [0,T] \to H^1(\omega) \times H^1(\omega;[0,1])$ satisfies properties (a)–(c) of Definition 5.1.5 and that for every $t \in [0,T]$*

$$\mathcal{F}(u(t),v(t)) \leq \mathcal{F}(u_0,v_0) - \frac{1}{2}\int_0^t |\partial_v^- \mathcal{F}|^2(u(s),v(s)) + \|\dot v(s)\|_{L^2}^2 \, \mathrm{d}s \\ + \int_0^t \mathcal{P}(u(s),v(s),\dot g(s))\, \mathrm{d}s\,. \quad (5.18)$$

Then, (u,v) also fulfills the energy balance (d) of Definition 5.1.5.

Proof. In order to prove the proposition we need to show the opposite inequality of (5.18). We exploit here the Riemann sum argument proposed in [55, Lemma 4.12]. Since by (5.18) the slope $|\partial_v^- \mathcal{F}|(u,v)$ is in $L^2(0,T)$, for every $t \in [0,T]$ there exists a sequence of subdivisions, denoted (by abuse of notation) by $0 = t_0^j < t_1^j < \cdots < t_{N_j}^j = t$ with $N_j \in \mathbb{N}$, such that

$$\lim_{j\to\infty} \max\{(t_{i+1}^j - t_i^j) : 0 \leq i \leq I_j - 1\} = 0\,,$$

and such that the piecewise constant functions

$$F_j(s) := \sum_{i=0}^{I_j} \mathbb{1}_{(t_i^j, t_{i+1}^j)}(s) |\partial_v^- \mathcal{F}|(u(t_i^j), v(t_i^j)) \quad (5.19)$$

converge to $|\partial_v^- \mathcal{F}|(u,v)$ strongly in $L^2(0,t)$.

By the quadratic structure of the functional $\mathcal{F}$, we can write

$$\begin{aligned} &\mathcal{F}(u(t_i^j), v(t_{i+1}^j)) \\ &= \mathcal{F}\Big(u(t_i^j), v(t_i^j) + (v(t_{i+1}^j) - v(t_i^j))\Big) \\ &= \mathcal{F}(u(t_i^j), v(t_i^j)) + \partial_v \mathcal{F}(u(t_i^j), v(t_i^j))[v(t_{i+1}^j) - v(t_i^j)] \\ &\quad + \frac{1}{2}\int_\omega (v(t_{i+1}^j) - v(t_i^j))^2 \nabla u(t_i^j)^\top A_1 \nabla u(t_i^j)\,\mathrm{d}x \\ &\quad + \frac{1}{2}\int_\omega (\nabla v(t_{i+1}^j) - \nabla v(t_i^j))^\top A_2 (\nabla v(t_{i+1}^j) - \nabla v(t_i^j))\,\mathrm{d}x \\ &\quad + \frac{1}{2}\int_\omega (v(t_{i+1}^j) - v(t_i^j))^2 h\,\mathrm{d}x \\ &\geq \mathcal{F}(u(t_i^j), v(t_i^j)) + \partial_v \mathcal{F}(u(t_i^j), v(t_i^j))[v(t_{i+1}^j) - v(t_i^j)] + \frac{c}{2}\|v(t_{i+1}^j) - v(t_i^j)\|_{H^1}^2\,, \end{aligned} \quad (5.20)$$

for some $c > 0$.

Reordering the terms in (5.20) and recalling Lemma 5.1.3, we get

$$\begin{aligned}
&\mathcal{F}\big(u(t_i^j), v(t_i^j)\big) \\
&\leq \mathcal{F}\big(u(t_i^j), v(t_{i+1}^j)\big) - \partial_v \mathcal{F}\big(u(t_i^j), v(t_i^j)\big)\big[v(t_{i+1}^j) - v(t_i^j)\big] - \frac{c}{2}\big\|v(t_{i+1}^j) - v(t_i^j)\big\|_{H^1}^2 \\
&\leq \mathcal{F}\big(u(t_i^j), v(t_{i+1}^j)\big) + \int_{t_i^j}^{t_{i+1}^j} |\partial_v^- \mathcal{F}|\big(u(t_i^j), v(t_i^j)\big) \frac{\big\|v(t_{i+1}^j) - v(t_i^j)\big\|_{L^2}}{(t_{i+1}^j - t_i^j)}\,\mathrm{d}s \\
&\quad - \frac{c}{2}\big\|v(t_{i+1}^j) - v(t_i^j)\big\|_{H^1}^2 .
\end{aligned} \tag{5.21}$$

For every $j \in \mathbb{N}$ and every $i \in \{0, \ldots, I_j - 1\}$, we have

$$\begin{aligned}
\mathcal{F}\big(u(t_i^j), v(t_{i+1}^j)\big) &= \mathcal{F}\big(u(t_i^j) + g(t_{i+1}^j) - g(t_i^j), v(t_{i+1}^j)\big) \\
&\quad - \int_{t_i^j}^{t_{i+1}^j} \partial_s \mathcal{E}\big(u(t_i^j) + g(s) - g(t_i^j), v(t_{i+1}^j)\big)\,\mathrm{d}s,
\end{aligned}$$

where

$$\begin{aligned}
&\partial_s \mathcal{E}\big(u(t_i^j) + g(s) - g(t_i^j), v(t_{i+1}^j)\big) \\
&= \partial_u \mathcal{E}\big(u(t_i^j) + g(s) - g(t_i^j), v(t_{i+1}^j)\big)\big[\dot{g}(s)\big] \\
&= \int_\omega b\big(u(t_i^j) + g(s) - g(t_i^j)\big)\dot{g}(s)\,\mathrm{d}x \\
&\quad + \int_\omega \big(v^2(t_{i+1}^j) + \eta\big)\nabla\big(u(t_i^j) + g(s) - g(t_i^j)\big)A_1\nabla\big(\dot{g}(s)\big)\,\mathrm{d}x \\
&= \mathcal{P}\big(u(t_i^j) + g(s) - g(t_i^j), v(t_{i+1}^j), \dot{g}(s)\big).
\end{aligned}$$

Next, we know that $u(t) \in \arg\min\{\mathcal{E}(u, v(t)) : u \in H^1(\omega), u = g(t) \text{ on } \partial\omega\}$ for every $t \in [0, T]$. Hence,

$$\int_\omega b\nabla u(t) \cdot \nabla\varphi\,\mathrm{d}x + \int_\omega (v^2(t) + \eta)\nabla u(t)^\top A_1 \nabla\varphi\,\mathrm{d}x = 0 \quad \text{for all } \varphi \in H_0^1(\omega).$$

As a consequence, if $w = g(t)$ on $\partial\omega$ we get

$$\begin{aligned}
&\mathcal{F}\big(w, v(t)\big) - \mathcal{F}\big(u(t), v(t)\big) \\
&= \int_\omega b\nabla\big(w + u(t)\big) \cdot \nabla\big(w - u(t)\big)\,\mathrm{d}x + \int_\omega \big(v^2(t) + \eta\big)\nabla\big(w + u(t)\big)^\top A_2 \nabla\big(w - u(t)\big)\,\mathrm{d}x \\
&= \int_\omega b\nabla\big(w - u(t)\big) \cdot \nabla\big(w - u(t)\big)\,\mathrm{d}x + \int_\omega \big(v^2(t) + \eta\big)\nabla\big(w - u(t)\big)^\top A_2 \nabla\big(w - u(t)\big)\,\mathrm{d}x \\
&\leq C\big\|w - u(t)\big\|_{H^1}^2 .
\end{aligned}$$

Choosing $t = t_{i+1}^j$ and $w = u(t_i^j) + g(t_{i+1}^j) - g(t_i^j)$ we can write

$$\mathcal{F}(u(t_i^j)+g(t_{i+1}^j)-g(t_i^j),v(t_{i+1}^j)) \le \mathcal{F}(u(t_{i+1}^j),v(t_{i+1}^j)) + C\|g(t_{i+1}^j)-g(t_i^j)\|_{H^1}^2 + C\|u(t_{i+1}^j)-u(t_i^j)\|_{H^1}^2. \quad (5.22)$$

Joining (5.21)–(5.22) we obtain

$$\begin{aligned} &\mathcal{F}(u(t_i^j),v(t_i^j)) \\ &\le \mathcal{F}(u(t_{i+1}^j),v(t_{i+1}^j)) + \int_{t_i^j}^{t_{i+1}^j} |\partial_v^- \mathcal{F}|(u(t_i^j),v(t_i^j)) \frac{\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}}{(t_{i+1}^j-t_i^j)}\,\mathrm{d}s \\ &\quad - \int_{t_i^j}^{t_{i+1}^j} \mathcal{P}(u(t_i^j)+g(s)-g(t_i^j),v(t_{i+1}^j),\dot g(s))\,\mathrm{d}s \\ &\quad - \frac{1}{2}\|v(t_{i+1}^j)-v(t_i^j)\|_{H^1}^2 + C\|g(t_{i+1}^j)-g(t_i^j)\|_{H^1}^2 + C\|u(t_{i+1}^j)-u(t_i^j)\|_{H^1}^2. \end{aligned} \quad (5.23)$$

We now estimate the last term in (5.23). By Lemma 5.1.8, we have that there exist $C>0$ and $q \gg 2$ independent of i and j such that

$$\|u(t_{i+1}^j)-u(t_i^j)\|_{H^1}^2 \le C\|g(t_{i+1}^j)-g(t_i^j)\|_{H^1}^2 + C\|v(t_{i+1}^j)-v(t_i^j)\|_{L^q}^2 .$$

By interpolation inequality, we can find $0<\alpha<1$ and $\bar q \gg 2$ such that

$$\|v(t_{i+1}^j)-v(t_i^j)\|_{L^q}^2 \le \|v(t_{i+1}^j)-v(t_i^j)\|_{L^{\bar q}}^{2\alpha} \|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}^{2(1-\alpha)} .$$

Applying a weighted Young inequality, we get that for every $\delta>0$ there exists $C_\delta>0$ such that

$$\|v(t_{i+1}^j)-v(t_i^j)\|_{L^q}^2 \le \delta\|v(t_{i+1}^j)-v(t_i^j)\|_{L^{\bar q}}^2 + C_\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}^2 .$$

In view of Sobolev embedding, we can continue with

$$\|v(t_{i+1}^j)-v(t_i^j)\|_{L^q}^2 \le C\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{H^1}^2 + C_\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}^2 .$$

Combining all the previous inequalities we get

$$\|u(t_{i+1}^j)-u(t_i^j)\|_{H^1}^2 \le C\|g(t_{i+1}^j)-g(t_i^j)\|_{H^1}^2 + C\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{H^1}^2 + C_\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}^2 . \quad (5.24)$$

Substituting (5.24) in (5.23) and choosing $\delta>0$ small enough so that $C\delta < \frac{C}{2}$, we obtain

$$\begin{aligned} &\mathcal{F}(u(t_i^j),v(t_i^j)) \\ &\le \mathcal{F}(u(t_{i+1}^j),v(t_{i+1}^j)) + \int_{t_i^j}^{t_{i+1}^j} |\partial_v^- \mathcal{F}|(u(t_i^j),v(t_i^j)) \frac{\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}}{(t_{i+1}^j-t_i^j)}\,\mathrm{d}s \\ &\quad - \int_{t_i^j}^{t_{i+1}^j} \mathcal{P}(u(t_i^j)+g(s)-g(t_i^j),v(t_{i+1}^j),\dot g(s))\,\mathrm{d}s \\ &\quad - \widetilde{C}\|v(t_{i+1}^j)-v(t_i^j)\|_{H^1}^2 + C\|g(t_{i+1}^j)-g(t_i^j)\|_{H^1}^2 + C_\delta\|v(t_{i+1}^j)-v(t_i^j)\|_{L^2}^2 , \end{aligned} \quad (5.25)$$

for some positive constants $C, \widetilde{C}$ independent of i and j.

Iterating inequality (5.25) for $i = 0, \ldots, I_j - 1$ and neglecting the terms with the H^1-norm of the phase field variable (which are negative), we finally arrive at

$$\mathcal{F}(u_0, v_0) \le \mathcal{F}(u(t), v(t)) + J_{1,j} - J_{2,j} + J_{3,j} + J_{4,j}$$

where

$$\begin{aligned}
J_{1,j} &:= \sum_{i=0}^{I_j-1} \int_{t_i^j}^{t_{i+1}^j} |\partial_v^- \mathcal{F}|(u(t_i^j), v(t_i^j)) \frac{\|v(t_{i+1}^j) - v(t_i^j)\|_{L^2}}{(t_{i+1}^j - t_i^j)} \, \mathrm{d}s \,, \\
J_{2,j} &:= \sum_{i=0}^{I_j-1} \int_{t_i^j}^{t_{i+1}^j} \mathcal{P}(u(t_i^j) + g(s) - g(t_i^j), v(t_{i+1}^j), \dot{g}(s)) \, \mathrm{d}s \,, \\
J_{3,j} &:= C \sum_{i=0}^{I_j-1} \|g(t_{i+1}^j) - g(t_i^j)\|_{H^1}^2 \,, \\
J_{4,j} &:= C \sum_{i=0}^{I_j-1} \|v(t_{i+1}^j) - v(t_i^j)\|_{L^2}^2 \,.
\end{aligned}$$

We now prove the following:

$$\lim_{j\to\infty} J_{1,j} = \int_0^t |\partial_v^- \mathcal{F}|(u(s), v(s)) \|\dot{v}(s)\|_{L^2} \, \mathrm{d}s \,, \tag{5.26}$$

$$\lim_{j\to\infty} J_{2,j} = \int_0^t \mathcal{P}(u(s), v(s), \dot{g}(s)) \, \mathrm{d}s \,, \tag{5.27}$$

$$\lim_{j\to\infty} J_{3,j} = \lim_{j\to\infty} J_{4,j} = 0 \,. \tag{5.28}$$

As for (5.26), we first rewrite $J_{1,j}$ as

$$J_{1,j} = \int_0^t F_j(s) V_j(s) \, \mathrm{d}s \,,$$

where F_j has been introduced in (5.19) and V_j is defined by

$$V_j(s) := \sum_{i=0}^{I_j-1} \mathbb{1}_{(t_i^j, t_{i+1}^j)}(s) \frac{\|v(t_{i+1}^j) - v(t_i^j)\|_{L^2}}{(t_{i+1}^j - t_i^j)} \quad \text{for all } s \in [0,t] \,.$$

We already know that, by the particular choice of the sequence of subdivisions of the interval $[0,t]$, the sequence F_j converges to $|\partial_v^- \mathcal{F}|(u,v)$ in $L^2(0,t)$. Hence, in order to get (5.27) it is enough to show that $V_j \rightharpoonup \|\dot{v}\|_{L^2}$ weakly in $L^2(0,t)$. Since $v \in H^1([0,T]; L^2(\omega))$, we have that $V_j(s) \to \|\dot{v}(s)\|_{L^2}$ for a.e. $s \in [0,t]$. Moreover, V_j is bounded in $L^2([0,t])$. Indeed,

$$\|V_j\|_{L^2(0,t)}^2 = \sum_{i=1}^{I_j-1} \int_{t_i^j}^{t_{i+1}^j} \left\| \frac{v(t_{i+1}^j) - v(t_i^j)}{t_{i+1}^j - t_i^j} \right\|_{L^2}^2 \mathrm{d}s \le \int_0^t \|\dot{v}(s)\|_{L^2}^2 \, \mathrm{d}s \,.$$

Therefore, we conclude that $V_j \rightharpoonup \|\dot{v}\|_{L^2}$ weakly in $L^2(0,t)$ and (5.26) holds true.

For the limit in (5.27) let us fix $s \in (0,t)$. For every $j \in \mathbb{N}$ let $s \in [t^j_{i_j}, t^j_{i_j+1})$, so that $t^j_{i_j} \to s$ and $t^j_{i_j+1} \to s$. Since $u \in C([0,T];H^1(\omega))$ and $v \in H^1([0,T];L^2(\omega))$, it is clear that $u(t^j_{i_j}) + g(s) - g(t^j_{i_j}) \to u(s)$ in $H^1(\omega)$ and $v(t^j_{i_j+1}) \to v(s)$ in $L^2(\omega)$. By Lemma 5.1.4

$$\mathcal{P}\big(u(t^j_i) + g(s) - g(t^j_i), v(t^j_{i+1}), \dot{g}(s)\big) \to \mathcal{P}\big(u(s), v(s), \dot{g}(s)\big) .$$

We get (5.27) by dominated convergence.

The limits (5.28) involving $J_{3,j}$ and $J_{4,j}$ follow, respectively, from the fact that the boundary datum $g \in AC([0,T];H^1(\omega))$ and the phase field $v \in H^1([0,T];L^2(\omega))$. This concludes the proof. □

5.2 Auxiliary Results

We collect here some technical results that will be useful in the next sections. We start with the weakly lower semi-continuity of our functional $\mathcal{F}$.

Lemma 5.2.1. *Let $u_m, u \in H^1(\omega)$ and $v_m, v \in H^1(\omega;[0,1])$ for every $m \in \mathbb{N}$. If $u_m \rightharpoonup u$ in $H^1(\omega)$ and $v_m \rightharpoonup v$ in $H^1(\omega)$, then*

$$\mathcal{E}(u,v) \le \liminf_{m\to\infty} \mathcal{E}(u_m,v_m) \quad \textit{and} \quad \mathcal{D}(u,v) \le \liminf_{m\to\infty} \mathcal{D}(u_m,v_m)$$

which yields

$$\mathcal{F}(u,v) \le \liminf_{m\to\infty} \mathcal{F}(u_m,v_m) .$$

Proof. The lower semi-continuity of $\mathcal{D}$ is obvious, by convexity. The lower semi-continuity of $\mathcal{E}$ follows for instance from [63, Theorem 7.5]. □

The elastic energy is even continuous with respect to the strong convergence in the first variable.

Lemma 5.2.2. *Let $u_m, u \in H^1(\omega)$ and $v_m, v \in H^1(\omega;[0,1])$ for all $m \in \mathbb{N}$. Assume that $u_m \to u$ and $v_m \rightharpoonup v$ in $H^1(\Omega)$. Then there holds*

$$\lim_{m\to\infty} \mathcal{E}(u_m,v_m) = \mathcal{E}(u,v)$$

Proof. Extract a subsequence (not relabeled) such that $v_m \to v$ and $\nabla u_m \to \nabla u$ a.e. in ω. Then

$$(v_m^2 + \eta)\nabla u_m^\top A_1 \nabla u_m \to (v_\infty + \eta)\nabla u^\top A_1 \nabla u \quad \text{a.e. in } \omega .$$

Since $0 \le v_m \le 1$ and $u_m \to u$ (strongly) in $H^1(\omega)$ we can apply the dominated convergence theorem and obtain $\mathcal{E}(u_m,v_m) \to \mathcal{E}(u,v)$. Because the limit is independent of the subsequence the assertion holds. □

We continue with a lower semi-continuity property of the slope $|\partial_v^- \mathcal{F}|$.

Lemma 5.2.3. *Let $u_m, u \in H^1(\omega)$ and $v_m, v \in H^1(\omega;[0,1])$ for all $m \in \mathbb{N}$. If $u_m \to u$ in $H^1(\omega)$ and $v_m \rightharpoonup v$ in $H^1(\omega)$, then*

$$|\partial_v^- \mathcal{F}|(u,v) \leq \liminf_{m\to\infty} |\partial_v^- \mathcal{F}|(u_m, v_m)\,. \tag{5.29}$$

Proof. Let us fix $\varphi \in H^1(\omega;[0,1])$ with $\varphi \leq 0$ and $\|\varphi\|_{L^2} \leq 1$. Without loss of generality, we assume that the lim inf in (5.29) is a limit and that $\nabla u_m \to \nabla u$ and $v_m \to v$ pointwise a.e. in ω. Then, by Lemma 5.1.3 we have that

$$\begin{aligned}
&\lim_{m\to\infty} |\partial_v^- \mathcal{F}|(u_m, v_m) \\
&\geq \liminf_{m\to\infty} -\partial_v \mathcal{F}(u_m, v_m)[\varphi] \\
&= \liminf_{m\to\infty} \int_\omega -v_m \varphi \nabla u_m A_1 \nabla u_m^\top \, \mathrm{d}x - \int_\omega \nabla v_m^\top A_2 \nabla \varphi - (1 - v_m)\varphi h \, \mathrm{d}x\,.
\end{aligned}$$

By (generalized) dominated convergence, for the first integral, and weak convergence, for the second integral, we get

$$\begin{aligned}
\lim_{m\to\infty} |\partial_v^- \mathcal{F}|(u_m, v_m) &\geq \int_\omega -v\varphi \nabla u^\top A_1 \nabla u \, \mathrm{d}x - \int_\omega \nabla v^\top A_2 \nabla \varphi - (1-v)\varphi h \, \mathrm{d}x \\
&= -\partial_v \mathcal{F}(u,v)[\varphi]\,.
\end{aligned}$$

Passing to the supremum with respect to φ in the previous inequality, we get (5.29). □

The Finally, we will prove the following minimality properties.

Lemma 5.2.4. *Let $g_m, g_\infty, u_m, u_\infty \in H^1(\omega)$ and let $v_m, v_\infty \in H^1(\omega;[0,1])$ for $m \in \mathbb{N}$. Assume that $g_m \to g_\infty$ and $u_m \rightharpoonup u_\infty$ in $H^1(\omega)$, $v_m \rightharpoonup v$ in $H^1(\omega)$, as well as*

$$u_m \in \arg\min\{\mathcal{E}(u, v_m) : u \in H^1(\omega) \text{ with } u = g_m \text{ on } \partial\omega\}\,. \tag{5.30}$$

Then

$$u_\infty \in \arg\min\{\mathcal{E}(u, v_\infty) : u \in H^1(\omega) \text{ with } u = g_\infty \text{ on } \partial\omega\} \tag{5.31}$$

and $u_m \to u_\infty$ strongly in $H^1(\omega)$.

Proof. Let $u \in H^1(\omega)$ be such that $u = g_\infty$ on $\partial\omega$, then $u - g_\infty + g_m = g_m$ on $\partial\omega$. By minimality, see (5.30), and by the lower semi-continuity of $\mathcal{E}$ from Lemma 5.2.1, we get

$$\mathcal{E}(u_\infty, v_\infty) \leq \liminf_{m\to\infty} \mathcal{E}(u_m, v_m) \leq \liminf_{m\to\infty} \mathcal{E}(u + g_m - g_\infty, v_m)\,. \tag{5.32}$$

From Lemma 5.2.2 we get $\lim_{m\to\infty} \mathcal{E}(u + g_m - g_\infty, v_m) = \mathcal{E}(u, v_\infty)$ from which (5.31) follows.

For the rest of the proof we show the strong convergence of (u_m). Replacing u by u_∞ in (5.32) we deduce

$$\lim_{m\to\infty} \mathcal{E}(u_m, v_m) = \mathcal{E}(u_\infty, v_\infty)\,.$$

Since A_1 fulfills (5.10), $\eta > 0$ and $0 \leq v_m \leq 1$, there exists $C > 0$ (independent of m) such that

$$\begin{aligned}\|\nabla(u_m - u_\infty)\|_{L^2}^2 &\leq C \int_\omega (v_m^2 + \eta)\nabla(u_m - u_\infty)^\top A_1 \nabla(u_m - u_\infty)\,\mathrm{d}x \\ &= C \int_\omega (v_m^2 + \eta)\nabla u_m^\top A_1 \nabla u_m + (v_m^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_\infty \\ &\quad - 2(v_m^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_m \,\mathrm{d}x\,.\end{aligned} \tag{5.33}$$

By convergence of the elastic energy we get

$$\int_\omega (v_m^2 + \eta)\nabla u_m^\top A_1 \nabla u_m \,\mathrm{d}x \to \int_\omega (v_\infty^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_\infty \,\mathrm{d}x\,,$$

and from the weak convergence of (v_m) we obtain

$$\int_\omega (v_m^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_\infty \,\mathrm{d}x \to \int_\omega (v_\infty^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_\infty \,\mathrm{d}x\,.$$

The dominated convergence theorem implies $(v_m^2 + \eta)\nabla u_\infty \to (v_\infty^2 + \eta)\nabla u_\infty$ in $L^2(\omega;\mathbb{R}^2)$, and together with the weak convergence of (∇u_m) in $L^2(\omega)$ we get

$$\int_\omega (v_m^2 + \eta)\nabla u_\infty A_1 \nabla u_m \,\mathrm{d}x \to \int_\omega (v_\infty^2 + \eta)\nabla u_\infty^\top A_1 \nabla u_\infty \,\mathrm{d}x\,.$$

Altogether, (5.33) yields $\nabla u_m \to \nabla u_\infty$ in $L^2(\omega, \mathbb{R}^2)$ and consequently $u_m \to u$ in $H^1(\omega)$. □

5.3 A one-step scheme

In this section we present a first time-discrete scheme, proposed in [102], converging to unilateral gradient flow, in the sense of Definition 5.1.5.

Given the time horizon $T > 0$, for every $k \in \mathbb{N}\backslash\{0\}$ we define the time step $\tau_k := \frac{T}{k}$. For every $i \in \{0, \dots, k\}$ we set the discrete time nodes $t_i^k := i\tau_k$ and we define recursively $u_i^k \in H^1(\omega)$ and $\tilde{v}_i^k, v_i^k \in H^1(\omega)$ as follows: for $i = 0$ let $u_0^k := u_0$ and $\tilde{v}_0^k = v_0^k := v_0$, while, for $i \geq 1$, we define

$$u_i^k := \arg\min\{\mathcal{E}(u, v_{i-1}^k) : u \in H^1(\omega),\, u = g(t_i^k) \text{ on } \partial\omega\}\,, \tag{5.34}$$

$$\tilde{v}_i^k := \arg\min\Big\{\mathcal{F}(u_i^k, v) + \frac{1}{2\tau_k}\|v - v_{i-1}^k\|_{L^2}^2 : v \in H^1(\omega)\Big\}\,. \tag{5.35}$$

$$v_i^k := \min\{\tilde{v}_i^k, v_{i-1}^k\}\,. \tag{5.36}$$

We notice that the solutions of the minimum problems (5.34) and (5.35) exist and are unique by the strict convexity of the involved functionals. In particular, by the usual truncation argument, we have that $0 \leq \tilde{v}_i^k \leq 1$ in ω whenever $0 \leq v_{i-1}^k \leq 1$ in ω. By induction, this is guaranteed by the restriction $0 \leq v_0 \leq 1$ on the initial condition.

Remark 5.3.1. We stress that the minimum problem (5.35) for the phase field variable is unconstrained, that is, we are not imposing any a priori irreversibility constraint of the form $v \le v^k_{i-1}$. The latter condition is instead imposed a posteriori by (5.36). Therefore, at the discrete level, the "non-increasing" phase field variable v^k_i does not satisfy any equilibrium condition, while the "unconstrained" phase field $\tilde v^k_i$ is not monotone, with respect to $i \in \mathbb{N}$. As discussed in [102], from a numerical viewpoint the approach described by (5.34)–(5.36) is computationally very convenient since, at every discrete time t^k_i, we have to solve a couple of unconstrained minimum problems for quadratic functionals.

We now show some consequences of (5.34)–(5.36).

Proposition 5.3.2. *For every $k \in \mathbb{N}$ and every $i \in \{1, \dots, k\}$ let u^k_i, $\tilde v^k_i$ and v^k_i be defined as in* (5.34)*–*(5.36)*. Then*

$$\frac{\|v^k_i - v^k_{i-1}\|_{L^2}}{\tau_k} = |\partial^-_v \mathcal{F}|(u^k_i, \tilde v^k_i)\,, \tag{5.37}$$

$$\begin{aligned}\partial_v \mathcal{F}(u^k_i, v^k_i)[v^k_i - v^k_{i-1}] &= \partial_v \mathcal{F}(u^k_i, \tilde v^k_i)[v^k_i - v^k_{i-1}] \\ &= -|\partial^-_v \mathcal{F}|(u^k_i, \tilde v^k_i)\|v^k_i - v^k_{i-1}\|_{L^2}\,.\end{aligned} \tag{5.38}$$

Proof. By minimality of $\tilde v^k_i$, we have that

$$\partial_v \mathcal{F}(u^k_i, \tilde v^k_i)[\varphi] + \frac{1}{\tau_k}\int_\omega (\tilde v^k_i - v^k_{i-1})\varphi \,\mathrm{d}x = 0 \quad \text{for all } \varphi \in H^1(\omega;[0,1])\,. \tag{5.39}$$

Then, by Lemma 5.1.3, by the density of $H^1(\omega;[0,1])$ in $L^2(\omega)$, and since $v^k_i - v^k_{i-1} = -[\tilde v^k_i - v^k_{i-1}]_-$, we have that

$$\begin{aligned}|\partial^-_v \mathcal{F}|(u^k_i, \tilde v^k_i) &= \sup\{-\partial_v \mathcal{F}(u^k_i, \tilde v^k_i)[\varphi] : \varphi \in H^1(\omega;[0,1]), \varphi \le 0, \|\varphi\|_{L^2} \le 1\} \\ &= \max\Big\{\frac{1}{\tau_k}\int_\omega (\tilde v^k_i - v^k_{i-1})\varphi \,\mathrm{d}x : \varphi \in L^2(\omega), \varphi \le 0, \|\varphi\|_{L^2} \le 1\Big\} \\ &= \frac{1}{\tau_k}\int_\omega [\tilde v^k_i - v^k_{i-1}]_- \frac{[\tilde v^k_i - v^k_{i-1}]_-}{\big\|[\tilde v^k_i - v^k_{i-1}]_-\big\|_{L^2}}\,\mathrm{d}x \\ &= \frac{1}{\tau_k}\big\|[\tilde v^k_i - v^k_{i-1}]_-\big\|_{L^2} \\ &= \frac{1}{\tau_k}\|v^k_i - v^k_{i-1}\|_{L^2}\,,\end{aligned}$$

which proves (5.37). In particular, since $(v^k_i - v^k_{i-1}) \in H^1(\omega;[0,1])$, we also deduce the second part of (5.38), i.e.

$$-\partial_v \mathcal{F}(u^k_i, \tilde v^k_i)[v^k_i - v^k_{i-1}] = |\partial^-_v \mathcal{F}|(u^k_i, \tilde v^k_i)\|v^k_i - v^k_{i-1}\|_{L^2}\,. \tag{5.40}$$

Let us now define $\omega_- := \{\tilde v^k_i \le v^k_{i-1}\}$ and $\omega_+ := \{\tilde v^k_i > v^k_{i-1}\}$. Then, we claim that

$$\partial_v \mathcal{F}(u^k_i, v^k_i)[\varphi] + \frac{1}{\tau_k}\int_\omega (v^k_i - v^k_{i-1})\varphi \,\mathrm{d}x = 0 \tag{5.41}$$

for every $\varphi \in H^1(\omega;[0,1])$ with $\varphi = 0$ on ω_+. Note that the partial derivative of $\mathcal{F}$ is computed in v_i^k and not in $\tilde{v}_i^k$, as in (5.39). Being $\varphi = 0$ on ω_+, we have

$$\int_{\omega_+} v_i^k \varphi (\nabla u_i^k)^\top A_1 \nabla u_i^k \,\mathrm{d}x + \int_{\omega_+} (\nabla v_i^k)^\top A_2 \nabla \varphi \,\mathrm{d}x \\ - \int_{\omega_+} (1 - v_i^k)\varphi \,\mathrm{d}x + \frac{1}{\tau_k}\int_{\omega_+} (v_i^k - v_{i-1}^k)\varphi h \,\mathrm{d}x = 0\,.$$

On the other hand, by (5.36), on ω_- we have $v_i^k = \tilde{v}_i^k$. Thus, in view of (5.39),

$$\begin{aligned} 0 &= \partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k)[\varphi] + \frac{1}{\tau_k}\int_\omega (\tilde{v}_i^k - v_{i-1}^k)\varphi \,\mathrm{d}x \\ &= \int_{\omega_-} v_i^k \varphi (\nabla u_i^k)^\top A_1 \nabla (u_i^k)\,\mathrm{d}x + \int_{\omega_-} (\nabla v_i^k)^\top A_2 \nabla\varphi \,\mathrm{d}x \\ &\quad - \int_{\omega_-} (1 - v_i^k)\varphi h \,\mathrm{d}x + \frac{1}{\tau_k}\int_{\omega_-} (v_i^k - v_{i-1}^k)\varphi \,\mathrm{d}x \end{aligned}$$

Hence (5.41) is proved.

Using now (5.39) and (5.41) with $\varphi = v_i^k - v_{i-1}^k$ we get

$$\begin{aligned} \partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k)[v_i^k - v_{i-1}^k] + \frac{1}{\tau_k}\int_\omega (\tilde{v}_i^k - v_{i-1}^k)(v_i^k - v_{i-1}^k)\,\mathrm{d}x = 0\,, \\ \partial_v \mathcal{F}(u_i^k, v_i^k)[v_i^k - v_{i-1}^k] + \frac{1}{\tau_k}\int_\omega (v_i^k - v_{i-1}^k)^2 \,\mathrm{d}x = 0\,. \end{aligned} \tag{5.42}$$

It is easy to see that

$$\int_\omega (\tilde{v}_i^k - v_{i-1}^k)(v_i^k - v_{i-1}^k)\,\mathrm{d}x = \int_\omega (v_i^k - v_{i-1}^k)^2\,\mathrm{d}x\,. \tag{5.43}$$

Combining (5.42)–(5.43), we obtain

$$\partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k)[v_i^k - v_{i-1}^k] = \partial_v \mathcal{F}(u_i^k, v_i^k)[v_i^k - v_{i-1}^k]\,,$$

which, together with (5.40), concludes the proof of the proposition. □

Remark 5.3.3. In view of the equilibrium condition (5.39), we could define $\partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k)$ as an element of $L^2(\omega)$ by the relation

$$\partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k)[\varphi] = -\frac{1}{\tau_k}\int_\omega (\tilde{v}_i^k - v_{i-1}^k)\varphi\,\mathrm{d}x \quad \text{for every } \varphi \in L^2(\omega)\,,$$

that is, $\partial_v \mathcal{F}(u_i^k, \tilde{v}_i^k) \cong -\frac{1}{\tau_k}(\tilde{v}_i^k - v_{i-1}^k)$ in $L^2(\omega)$.

We now define the following interpolation functions for every $k \in \mathbb{N}$ and $i \in \{1, \dots, k\}$:

$$v_k(t) := v_{i-1}^k + \frac{v_i^k - v_{i-1}^k}{\tau_k}(t - t_{i-1}^k), \quad \underline{u}_k(t) := u_{i-1}^k, \quad \underline{v}_k(t) := v_{i-1}^k$$

for every $t \in [t^k_{i-1}, t^k_i)$, and

$$\bar{u}_k(t) := u^k_i, \quad \bar{v}_k(t) := v^k_i, \quad \tilde{v}_k(t) := \tilde{v}^k_i, \quad t_k(t) := t^k_i\,,$$

for every $t \in (t^k_{i-1}, t^k_i]$. Next, we study compactness and energy balance for the sequences introduced just above.

Proposition 5.3.4. *The following facts hold:*

(a) The sequence (v_k) is bounded in $L^\infty([0,T]; H^1(\omega))$ and in $H^1([0,T]; L^2(\omega))$;

(b) The sequences $(\bar{v}_k)$, $(\tilde{v}_k)$, and $(\underline{v}_k)$ are bounded in $L^\infty([0,T]; H^1(\omega))$;

(c) The sequences $(\bar{u}_k)$ and $(\underline{u}_k)$ are bounded in $L^\infty([0,T]; H^1(\omega))$;

(d) For every $t \in [0,T]$ we have

$$\bar{u}_k(t) \in \operatorname{arg\,min}\Big\{\mathcal{E}\big(u, \underline{v}_k(t)\big) : u \in H^1(\omega), u = g\big(t_k(t)\big) \text{ on } \partial\omega\Big\}\,;$$

(e) There exists a constant $C > 0$ (depending only on A_1) such that for every $t \in [0,T]$

$$\begin{aligned}\mathcal{F}\big(\bar{u}_k(t), \underline{v}_k(t)\big) \le \mathcal{F}(u_0, v_0) - \frac{1}{2}\int_0^{t_k(t)} \big\|\dot{v}_k(s)\big\|^2_{L^2} + |\partial^-_v \mathcal{F}|^2\big(\bar{u}_k(s), \tilde{v}_k(s)\big)\,\mathrm{d}s \\ + \int_0^{t_k(t)} \mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s)\big)\,\mathrm{d}s + C\sum_{i=1}^{I_t}\big\|g(t^k_i) - g(t^k_{i-1})\big\|^2_{H^1}\,,\end{aligned} \tag{5.44}$$

where $I_t = \min\{I \in \mathbb{N} \mid I \ge \frac{t}{\tau_k}\}$. In particular the energy $\mathcal{F}(\bar{u}_k(t), \underline{v}_k(t))$ is uniformly bounded with respect to t and k.

Proof. We will start proving the energy estimate (e). Let us fix $k \in \mathbb{N}$, $t \in (0,T]$, and $i \in \{1, \dots, k\}$ such that $t \in (t^k_{i-1}, t^k_i)$. By convexity of $v \mapsto \mathcal{F}(u^k_i, v)$, we have that

$$\begin{aligned}\mathcal{F}(u^k_i, v^k_{i-1}) &\ge \mathcal{F}(u^k_i, v^k_i) + \partial_v \mathcal{F}(u^k_i, v^k_i)[v^k_{i-1} - v^k_i] \\ &= \mathcal{F}(u^k_i, v^k_i) - \tau_k \partial_v \mathcal{F}(u^k_i, v^k_i)\big[\dot{v}_k(t)\big]\,.\end{aligned} \tag{5.45}$$

Recalling Proposition 5.3.2, we can continue in (5.45) with

$$\begin{aligned}\mathcal{F}(u^k_i, v^k_{i-1}) &\ge \mathcal{F}(u^k_i, v^k_i) + \tau_k |\partial^-_v \mathcal{F}|(u^k_i, \tilde{v}^k_i)\big\|\dot{v}_k(t)\big\|_{L^2} \\ &= \mathcal{F}(u^k_i, v^k_i) + \frac{\tau_k}{2}\Big(\big\|\dot{v}_k(t)\big\|^2_{L^2} + |\partial^-_v \mathcal{F}|^2(u^k_i, \tilde{v}^k_i)\Big) \\ &= \mathcal{F}(u^k_i, v^k_i) + \frac{1}{2}\int_{t^k_{i-1}}^{t^k_i} \big\|\dot{v}_k(s)\big\|^2_{L^2} + |\partial^-_v \mathcal{F}|^2\big(\bar{u}_k(s), \tilde{v}_k(s)\big)\,\mathrm{d}s\,.\end{aligned} \tag{5.46}$$

Since $u_{i-1}^k + g(t_i^k) - g(t_{i-1}^k) = g(t_i^k)$ on $\partial\omega$, in view of the minimality (5.34) of u_i^k and of the quadratic structure of the elastic energy $\mathcal{E}$, we have that

$$\begin{aligned}\mathcal{E}(u_i^k, v_{i-1}^k) &\le \mathcal{E}\big(u_{i-1}^k + g(t_i^k) - g(t_{i-1}^k), v_{i-1}^k\big)\\ &= \mathcal{E}\big(u_{i-1}^k, v_{i-1}^k\big) + \mathcal{E}\big(g(t_i^k) - g(t_{i-1}^k), v_{i-1}^k\big)\\ &\quad + \int_\omega f u_{i-1}^k\big(g(t_i^k) - g(t_{i-1}^k)\big)\,\mathrm{d}x\\ &\quad + \int_\omega \big((v_{i-1}^k)^2 + \eta\big)(\nabla u_{i-1}^k)^\top A_1 \nabla\big(g(t_i^k) - g(t_{i-1}^k)\big)\,\mathrm{d}x\,.\end{aligned} \tag{5.47}$$

The second term is estimated, with the help of (5.12), by

$$\mathcal{E}\big(g(t_i^k) - g(t_{i-1}^k), v_{i-1}^k\big) \le C\big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2\,,$$

while the last two terms are rewritten as

$$\begin{aligned}&\int_\omega f u_{i-1}^k\big(g(t_i^k) - g(t_{i-1}^k)\big)\,\mathrm{d}x + \int_\omega \big((v_{i-1}^k)^2 + \eta\big)(\nabla u_{i-1}^k)^\top A_1 \nabla\big(g(t_i^k) - g(t_{i-1}^k)\big)\,\mathrm{d}x\\ &= \int_{t_{i-1}^k}^{t_i^k}\Big(\int_\omega f u_{i-1}^k \dot g(s)\,\mathrm{d}x + \int_\omega \big((v_{i-1}^k)^2 + \eta\big)(\nabla u_{i-1}^k)^\top A_1 \nabla \dot g(s)\,\mathrm{d}x\Big)\,\mathrm{d}s\\ &= \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot g(s)\big)\,\mathrm{d}s\,.\end{aligned}$$

Hence, (5.47) gives

$$\mathcal{F}(u_i^k, v_{i-1}^k) \le \mathcal{F}(u_{i-1}^k, v_{i-1}^k) + \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot g(s)\big)\,\mathrm{d}s + C\big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2\,. \tag{5.48}$$

Combining inequalities (5.46) and (5.48) and iterating over i, we deduce (5.44).

Property (d) follows simply from the construction of u_i^k and the definition of $\bar u_k$ and $\underline{v}_k$. It remains to prove compactness and the uniform bound of the energy $\mathcal{F}(\bar u_k(t), \underline{v}_k(t))$. By minimality of u_i^k, for every $k \in \mathbb{N}$ and every $i \in \{1, \dots, k\}$, and by (5.12) we can estimate

$$\|u_i^k\|_{H^1(\omega)}^2 \le \mathcal{E}(u_i^k, v_{i-1}^k) \le \mathcal{E}\big(g(t_i^k), v_{i-1}^k\big) \le C\big\|g(t_i^k)\big\|_{H^1(\omega)}^2 \le C'\,,$$

for some positive constant C', independent of the indices k and i. This concludes the proof of (c). Using the fact that $\underline{v}_k(t)$ takes values in $[0,1]$ and that $\underline{u}_k$ is bounded in $L^\infty([0,T]; H^1(\omega))$, we easily deduce that

$$\mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot g(s)\big) = \int_\omega \big(\underline{v}_k^2(s) + \eta\big)\big(\nabla \underline{u}_k(s)\big)^\top A_1 \nabla \dot g(s)\,\mathrm{d}x \le C\big\|\dot g(s)\big\|_{H^1(\omega)}\,. \tag{5.49}$$

Since $g \in AC([0,T]; H^1(\omega))$ we have

$$\int_0^{t_k(t)} \mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot g(s)\big)\,\mathrm{d}s \le C\,,$$

and

$$\sum_{i=1}^{I_t} \|g(t_i^k) - g(t_{i-1}^k)\|_{H^1}^2 \le \left(\sum_{i=1}^{k} \|g(t_i^k) - g(t_{i-1}^k)\|_{H^1} \right)^2 \le C \, .$$

These bounds, together with (5.44), imply that $\mathcal{F}(\bar{u}_k(t), \underline{v}_k(t))$ is uniformly bounded and that v_k is bounded in $H^1([0,T]; L^2(\omega))$. Since the energy is bounded, the phase field sequences v_k, $\bar{v}_k$, and $\underline{v}_k$ (all taking value v_i^k in the points t_i^k) are bounded in $L^\infty([0,T]; H^1(\omega))$. By minimality of $\tilde{v}_i^k$ we have $\mathcal{F}(u_i^k, \tilde{v}_i^k) \le \mathcal{F}(u_i^k, v_i^k)$, hence the sequence $\tilde{v}_k$ is bounded in $L^\infty([0,T]; H^1(\omega))$ as well. □

We are now ready to prove the convergence of the one-step scheme (5.34)–(5.36) towards a unilateral L^2-gradient flow.

Theorem 5.3.5. *There exists a subsequence, not relabelled, of the pair $(\bar{u}_k, v_k)$ such that*

(a) $v_k \rightharpoonup v$ *in* $H^1([0,T]; L^2(\omega))$*;*

(b) $v_k(t) \rightharpoonup v(t)$, $\bar{v}_k(t) \rightharpoonup v(t)$, $\tilde{v}_k(t) \rightharpoonup v(t)$, $\underline{v}_k(t) \rightharpoonup v(t)$ *in* $H^1(\omega)$ *for every* $t \in [0,T]$*;*

(c) $\bar{u}_k(t) \to u(t)$ *in* $H^1(\omega)$ *for every* $t \in [0,T]$*;*

(d) (u,v) *is a unilateral* L^2*-gradient flow for* $\mathcal{F}$*, in the sense of Definition 5.1.5.*

Proof. In view of Proposition 5.3.4 (a) and (c), we get (a) for some $v \in H^1([0,T]; L^2(\omega))$ and $\bar{u}_k(t) \rightharpoonup u(t)$ in $H^1(\omega)$ for some $u(t) \in H^1(\omega)$ for every $t \in [0,T]$. Identifying $v \in H^1([0,T]; L^2(\omega))$ with its continuous representative, we can write

$$v_k(t) = v_0 + \int_0^t \dot{v}_k(s)\,\mathrm{d}s \quad \text{and} \quad v(t) = v_0 + \int_0^t \dot{v}(s)\,\mathrm{d}s \quad \text{for all } t \in [0,T].$$

Hence $v_k(t) \rightharpoonup v(t)$ in $L^2(\omega)$ for every $t \in [0,T]$; as $v_k(t)$ is uniformly bounded in $H^1(\omega)$ we actually have $v_k(t) \rightharpoonup v(t)$ in $H^1(\omega)$. It is easy to check that v is non-increasing in time and takes values in the interval $[0,1]$. Remembering the definition v_k, $\underline{v}_k$ and $\bar{v}_k$ we can write

$$\bar{v}_k(t) = v_0 + \int_0^{t_k(t)} \dot{v}_k(s)\,\mathrm{d}s \, .$$

Note that the integrand is still $\dot{v}_k$. Since $t_k(t) \to t$, for every $t \in [0,T]$, we have $\bar{v}_k(t) \rightharpoonup v(t)$ in $H^1(\omega)$ for every $t \in [0,T]$. In a similar way we deduce that $\underline{v}_k(t) \rightharpoonup v(t)$ in $H^1(\omega)$ for every $t \in [0,T]$. We also notice that, in view of the minimum problem (5.35),

$$\|\tilde{v}_k(t) - \underline{v}_k(t)\|_{L^2}^2 \le 2\tau_k \mathcal{F}(\bar{u}_k(t), \underline{v}_k(t)) \le C\tau_k$$

for some positive constant C independent of k. Therefore, $\tilde{v}_k(t) \rightharpoonup v(t)$ in $H^1(\omega)$ for every $t \in [0,T]$ and the proof of (b) is complete.

Recalling Proposition 5.3.4 (d) and taking into account that $\underline{v}_k(t) \rightharpoonup v(t)$ and $g(t_k(t)) \to g(t)$ in $H^1(\omega)$ for every $t \in [0,T]$, Lemma 5.2.4 implies

$$u(t) \in \arg\min\Big\{\mathcal{E}(u, v(t)) : u \in H^1(\omega), u = g(t) \text{ on } \partial\omega\Big\}.$$

Furthermore, from Lemma 5.2.4 we get that $\bar{u}_k(t) \to u(t)$ in $H^1(\omega)$ for every $t \in [0,T]$. At this point, using the time regularity of v and g, by Lemma 5.1.8 (or simply by Lemma 5.2.4) we deduce that $u \in C([0,T]; H^1(\omega))$. Finally, let us see that $\underline{u}_k(t) \to u(t)$ in $H^1(\omega)$ for every $t \in [0,T]$. Indeed, it is enough to notice that $\underline{u}_k(t) = \bar{u}_k(t - \tau_k)$ satisfies

$$\underline{u}_k(t) \in \arg\min\{\mathcal{E}(u, \underline{v}_k(t - \tau_k)) :\ u \in H^1(\omega),\ u = g(t_k(t) - \tau_k) \text{ on } \partial\omega\}\,.$$

Arguing as above, we conclude the proof of (c) again by Lemma 5.2.4 and the uniqueness of minimizers.

To complete the proof, it remains to show the energy balance (d) of Definition 5.1.5. To this end, we will pass to the limit in the energy estimate (5.44). Since $\bar{u}_k(t) \to u(t)$ in $H^1(\omega)$ and $\underline{v}_k(t) \rightharpoonup v(t)$ in $H^1(\omega)$, by Lemma 5.2.1 and (5.44) we get

$$\begin{aligned}
&\mathcal{F}(u(t), v(t)) \\
&\le \liminf_{k\to\infty} \mathcal{F}(\bar{u}_k(t), \underline{v}_k(t)) \\
&\le \limsup_{k\to\infty}\Big(\mathcal{F}(u_0, v_0) - \frac{1}{2}\int_0^{t_k(t)} \big\|\dot{v}_k(s)\big\|_{L^2}^2 + |\partial_v^- \mathcal{F}|^2(\bar{u}_k(s), \tilde{v}_k(s))\,\mathrm{d}s\Big) \\
&\quad + \limsup_{k\to\infty} \int_0^{t_k(t)} \mathcal{P}(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s))\,\mathrm{d}s + \limsup_{k\to\infty} \sum_{i=1}^{k} \big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2 \\
&\le \mathcal{F}(u_0, v_0) - \liminf_{k\to\infty} \frac{1}{2}\int_0^{t_k(t)} \big\|\dot{v}_k(s)\big\|_{L^2}^2\,\mathrm{d}s - \liminf_{k\to\infty} \frac{1}{2}\int_0^{t_k(t)} |\partial_v^- \mathcal{F}|^2(\bar{u}_k(s), \tilde{v}_k(s))\,\mathrm{d}s \\
&\quad + \limsup_{k\to\infty} \int_0^{t_k(t)} \mathcal{P}(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s))\,\mathrm{d}s + \limsup_{k\to\infty} \sum_{i=1}^{k} \big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2\,.
\end{aligned}$$

Since $v_k \rightharpoonup v$ in $H^1([0,T]; L^2(\omega))$ and $t_k(t) \to t$ we get by the weakly lower semicontinuity of the norm

$$-\liminf_{k\to\infty} \int_0^{t_k(t)} \|\dot{v}_k(s)\|_{L^2}^2\,\mathrm{d}s \le -\int_0^t \|\dot{v}(s)\|_{L^2}^2\,\mathrm{d}s.$$

Since $\bar{u}_k \to u$ and $\tilde{v}_k \rightharpoonup v$ pointwise in $[0,T]$, applying Fatou's lemma and Lemma 5.2.3 we obtain

$$-\liminf_{k\to\infty} \int_0^{t_k(t)} |\partial_v^- \mathcal{F}|^2(\bar{u}_k(s), \tilde{v}_k(s))\,\mathrm{d}s \le -\int_0^t |\partial_v^- \mathcal{F}|^2(u(s), v(s))\,\mathrm{d}s\,.$$

Since $\underline{u}_k(s) \to u(s)$ and $\underline{v}_k(s) \rightharpoonup v(s)$ in $H^1(\omega)$ for all $s \in [0,T]$, from Lemma 5.1.4 we know that $\mathcal{P}(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s)) \to \mathcal{P}(u(s), v(s), \dot{g}(s))$ for all $s \in [0,T]$. Since $0 \le \underline{v}_k \le 1$ and $\underline{u}_k$ is bounded in $L^\infty([0,T]; H^1(\omega))$ we get (as in (5.49))

$$\mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s)\big) \le C \big\|\dot{g}(s)\big\|_{H^1} \le C' \quad \text{for all } s \in [0,T].$$

Hence, by dominated convergence,

$$\limsup_{k\to\infty} \int_0^{t_k(t)} \mathcal{P}\big(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s)\big)\, \mathrm{d}s \le \int_0^t \mathcal{P}\big(u(s), v(s), \dot{g}(s)\big)\, \mathrm{d}s\,.$$

Finally, being $g \in AC([0,T]; H^1(\omega))$, for every $\varepsilon > 0$ we have $\|g(t_i^k) - g(t_{i-1}^k)\|_{H^1} \le \varepsilon$ for every $i \in \{1, \dots, k\}$ and every $k \in \mathbb{N}$ sufficiently large. Hence,

$$\sum_{i=1}^k \big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2 \le \epsilon \sum_{i=1}^k \|g(t_i^k) - g(t_{i-1}^k)\|_{H^1} \le \epsilon \int_0^T \|\dot{g}(s)\|_{H^1}\, \mathrm{d}s \le C\epsilon\,,$$

and therefore,

$$\limsup_{k\to\infty} \sum_{i=1}^k \big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2 = 0\,.$$

In conclusion

$$\mathcal{F}\big(u(t), v(t)\big) \le \mathcal{F}(u_0, v_0) - \frac{1}{2}\int_0^t \big\|\dot{v}(s)\big\|_{L^2}^2 + |\partial_v^- \mathcal{F}|^2\big(u(s), v(s)\big)\, \mathrm{d}s + \int_0^t \mathcal{P}\big(u(s), v(s), \dot{g}(s)\big)\, \mathrm{d}s\,.$$

The opposite inequality follows by Proposition 5.1.9. This concludes the proof. □

5.4 The Space Discrete Setting

In this section we present a finite element discretization for our unilateral L^2-gradient flow. Our aim is twofold: to provide a space-discrete (finite element) version of the unilateral L^2-gradient flow and then to show that its space-continuous limit is again a unilateral L^2-gradient flow, in the sense of Definition 5.1.5.

First, in Section 5.4.1, we will introduce a discrete energy $\mathcal{F}_h$ defined in discretized spaces $\mathcal{V}_h$ and $\mathcal{U}_h$ (h being the mesh size); the evolution will then be defined, in Section 5.4.2, using again a time discrete approach in which the time-incremental problem is provided by a finite-step algorithm. We stress here that this finite-step algorithm is flexible enough to cover every stopping criterion, including those employed in the numerical simulations of Chapter 6.

Finally, in Section 5.4.3 we will show that, as the mesh size vanishes, the finite element evolutions converge to a (space-continuous) unilateral L^2-gradient flow, in the sense of Definition 5.1.5.

5.4.1 A Finite Element Discretization

First, let us describe the space-discrete setting we are considering in this section. For simplicity let $\omega \subset \mathbb{R}^2$ be polyhedral, and let $\{\mathcal{T}_h\}_{h>0}$ be a family of acute-angle triangulations of ω. Since ω is polyhedral we can assume that the triangulations are exact, and hence we do not have to take care about any geometric errors. We will denote by K the (triangular) elements and assume that $\mathrm{diam}(K) \leq h$.

Furthermore, we denote by Δ_h the set of all the vertices of $\mathcal{T}_h$ and we set $N_h := \#\Delta_h$.

We denote by $\mathcal{U}_h$ and $\mathcal{V}_h$ the sets of continuous P_1 finite elements functions on ω discretizing, respectively, the function spaces $H^1(\omega)$ and $H^1(\omega; [0,1])$.

In what follows, we will consider in $\mathcal{V}_h$ the basis of shape functions $\{\xi_l\}_{l=1}^{N_h}$, where

$$\xi_l(x_m) = \delta_{lm} \qquad \text{for every } x_m \in \Delta_h\,, \tag{5.50}$$

being δ_{lm} the Kronecker delta. Accordingly, we introduce the Lagrangian interpolant $\Pi_h \colon C(\bar{\omega}) \to \mathcal{V}_h$, i.e., the linear operator such that

$$\Pi_h(\varphi)(x_l) = \varphi(x_l) \qquad \text{for every } \varphi \in C(\bar{\omega}) \text{ and } x_l \in \Delta_h\,.$$

Note that, being $\mathcal{T}_h$ an acute-angle mesh, the basis $\{\xi_l\}_{l=1}^{N_h}$ satisfies the stiffness condition

$$\int_\omega \nabla \xi_l^\top A_2 \nabla \xi_m \,\mathrm{d}x \leq 0 \qquad \text{for every } l, m \in \{1, \dots, N_h\}, l \neq m\,. \tag{5.51}$$

For A_2 being the identity, this condition is satisfied for $\mathcal{T}_h$ being an acute-angle mesh, and it is a natural assumption in order to have a discrete maximum principle in $\mathcal{V}_h$ (e.g., [45, 101]) and, in turn, to ensure that, in the evolution, phase field functions will take values in $[0,1]$ (see Proposition 5.4.15).

Remark 5.4.1. Having in mind that the matrix A_2 corresponds to a metric tensor of a Riemannian manifold from Chapter 3 multiplied with a positive function, we get by coordinate transformation, that condition (5.51) is fulfilled if the triangulation is acute in the Riemannian space. Precisely, in the notation of the previous chapter the tangential gradient is defined for all $\hat{u} \in C^1(S)$ by

$$\nabla_\tau \hat{u} = (\nabla \tilde{u} - \langle \nabla \tilde{u}, g^3 \rangle g^3)|_S$$

where $\tilde{u}$ is an extension of $\hat{u}$ to $\Phi(\omega_\rho)$, which is the surface applied with a thickness ρ. Then, it is easy to compute by coordinate transformation that (5.51) is equivalent to

$$\int_{\phi(\omega)} \nabla_\tau (\xi_l \circ \phi^{-1})^\top \cdot \nabla_\tau (\xi_k \circ \phi^{-1}) \,\mathrm{d}x \quad \text{for all } l, m \in \{1, \dots, N_h\}, l \neq m\,.$$

In general, $\mathcal{U}_h$ and $\mathcal{V}_h$ will be endowed with the usual H^1-norms. However, we will employ in $\mathcal{V}_h$ a further norm given by

$$\|v\|_{\mathcal{V}_h} := \left(\int_\omega |\Pi_h(v^2)| \,\mathrm{d}x \right)^{1/2} \quad \text{for every } v \in \mathcal{V}_h\,.$$

Using the definition of the basis $\{\xi_l\}_{l=1}^{N_h}$, it is easy to check that $\|\cdot\|_{\mathcal{V}_h}$ is a norm in $\mathcal{V}_h$. Moreover, we have the following property.

Lemma 5.4.2. *For every $v \in \mathcal{V}_h$ we have $\|v\|_{L^2} \leq \|v\|_{\mathcal{V}_h}$.*

Proof. Let $\{x_l\}_{l=1}^{N_h}$ be the vertices of the triangulation $\mathcal{T}_h$. By the convexity of the quadratic function and the fact that $\sum_{l=1}^{N_h} \xi_l = 1$ with $0 \leq \xi_l \leq 1$, for every $l \in \{1, \ldots, N_h\}$, we have

$$v^2 = \left(\sum_{l=1}^{N_h} v(x_l) \xi_l \right)^2 \leq \sum_{l=1}^{N_h} v^2(x_l) \xi_l = \Pi_h(v^2) \,.$$

The assertion follows by integration over ω. □

Remark 5.4.3. Note that on each triangle K, denoting by x_i for $i = 1, 2, 3$ the vertices of K, we have

$$\int_K \Pi_h(v^2)\, \mathrm{d}x = \sum_{i=1}^{3} v^2(x_i) \Big(\int_K \xi_i \, \mathrm{d}x \Big) = \sum_{i,j=1}^{3} v(x_i) v(x_j) D_{ij}$$

where D is the diagonal matrix with entries $D_{ij} = \delta_{ij}(\int_K \xi_i \, \mathrm{d}x)$. Without the interpolation operator Π_h we would have the L^2-norm

$$\begin{aligned} \int_K v^2 \, \mathrm{d}x &= \int_K \Big(\sum_{i=1}^{3} v(x_i) \xi_i \Big)^2 \mathrm{d}x \\ &= \sum_{i,j=1}^{3} v(x_i) v(x_j) \Big(\int_K \xi_i \xi_j \, \mathrm{d}x \Big) = \sum_{i,j=1}^{3} v(x_i) v(x_j) A_{ij} \end{aligned}$$

where A is, in general, a full matrix. In practice, employing the operator Π_h results in a simpler numerical integration formula for the quadratic function v^2 and, in our case, for the elastic energy (see below).

In our finite element setting we introduce the discrete counterparts of the stored elastic energy (5.11) and of the dissipated energy (5.13): for every $u \in \mathcal{U}_h$ and every $v \in \mathcal{V}_h$ we set, respectively,

$$\begin{aligned} \mathcal{E}_h(u, v) &:= \frac{1}{2} \int_\omega b|u|^2 \, \mathrm{d}x + \frac{1}{2} \int_\omega (\Pi_h(v^2) + \eta)\, \nabla u^\top A_1 \nabla u \, \mathrm{d}x \,, \\ \mathcal{D}_h(v) &:= \frac{1}{2} \int_\omega \nabla v^\top A_2 \nabla v \, \mathrm{d}x + \frac{1}{2} \int_\omega \Pi_h\big((1 - v)^2\big) h \, \mathrm{d}x \,. \end{aligned}$$

As in (5.14), the *discrete total energy* is the sum of $\mathcal{E}_h$ and $\mathcal{D}_h$. Hence, for $u \in \mathcal{U}_h$ and $v \in \mathcal{V}_h$, we define

$$\mathcal{F}_h(u, v) := \mathcal{E}_h(u, v) + \mathcal{D}_h(v) \,.$$

Remark 5.4.4. In general the energy functional $\mathcal{F}$ is discretized simply by taking its restriction to the finite element spaces, i.e., by setting $\mathcal{F}_h := \mathcal{F}|_{\mathcal{U}_h \times \mathcal{V}_h}$. Here, instead, following the ideas of [2, 16], we redefine $\mathcal{F}_h$ using also the projection operator Π_h. In this way we ensure that during the evolution the phase field function $v \in \mathcal{V}_h$ will take values in $[0, 1]$ (see Proposition 5.4.15).

We notice that, as in (5.16), for every $u \in \mathcal{U}_h$ and every $v, \varphi \in \mathcal{V}_h$ there exists the derivative $\partial_v \mathcal{F}_h$ of $\mathcal{F}_h$ with respect to v. By linearity of Π_h, it reads

$$\partial_v \mathcal{F}_h(u,v)[\varphi] = \int_\omega \Pi_h(v\varphi)\, \nabla u^\top A_1 \nabla u \,\mathrm{d}x + \int_\omega \nabla v^\top A_2 \nabla \varphi \,\mathrm{d}x - \int_\omega \Pi_h((1-v)\varphi) h \,\mathrm{d}x\,.$$

Similarly to Definition 5.1.1, we introduce the *discrete unilateral L^2-slope* of $\mathcal{F}_h$.

Definition 5.4.5. For every $u \in \mathcal{U}_h$ and every $v \in \mathcal{V}_h$, we define the discrete unilateral L^2-slope of $\mathcal{F}_h$ as

$$|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u,v) := \limsup_{\substack{z \to v \\ z \in \mathcal{V}_h, z \leq v}} \frac{[\mathcal{F}_h(u,v) - \mathcal{F}_h(u,z)]_+}{\|z - v\|_{\mathcal{V}_h}}\,.$$

With the argument used in Lemma 5.1.3, we can show the following.

Lemma 5.4.6. *For every $h > 0$, every $u \in \mathcal{U}_h$, and every $v \in \mathcal{V}_h$,*

$$|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u,v) = \sup\{-\partial_v \mathcal{F}_h(u,v)[\varphi] : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1\}\,. \tag{5.52}$$

Remark 5.4.7. Note that here the normalization in (5.52) is with respect to the norm $\|\cdot\|_{\mathcal{V}_h}$.

We now prove a lower semi-continuity property of the slope $|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}$ similar to Lemma 5.2.3.

Lemma 5.4.8. *Fix $h > 0$. If $u_m \to u$ in $\mathcal{U}_h$ and $v_m \to v$ in $\mathcal{V}_h$, then*

$$|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u,v) \leq \liminf_{m \to \infty} |\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_m, v_m)\,.$$

Proof. The proof can be done as in Lemma 5.2.3. □

Following the steps of Section 5.1, we introduce the space-discrete counterpart of the power of external forces (5.17). For every $u, z \in \mathcal{U}_h$ and every $v \in \mathcal{V}_h$ we set

$$\mathcal{P}_h(u,v,z) := \int_\omega f u z \,\mathrm{d}x + \int_\omega (\Pi_h(v^2) + \eta)\, \nabla u^\top A_1 \nabla z \,\mathrm{d}x\,.$$

We are now ready to give the definition of *finite-dimensional unilateral L^2-gradient flow.*

Definition 5.4.9. Let $h > 0$, $T > 0$, and let $g \in AC([0,T];\mathcal{U}_h)$. Let $u_0 \in \mathcal{U}_h$ with $u_0 = g(0)$ on $\partial\omega$ and let $v_0 \in \mathcal{V}_h$ be such that $0 \leq v_0 \leq 1$ and

$$u_0 \in \arg\min\{\mathcal{E}_h(u, v_0) : u \in \mathcal{U}_h \text{ with } u = g(0) \text{ on } \partial\omega\}\,. \tag{5.53}$$

We say that a pair $(u,v)\colon [0,T] \to \mathcal{U}_h \times \mathcal{V}_h$ is a *finite-dimensional unilateral L^2-gradient flow* for the energy $\mathcal{F}_h$ with initial condition (u_0, v_0) and boundary condition g if the following properties are satisfied:

(a) *Time regularity*: $u \in C([0,T];\mathcal{U}_h)$ and $v \in H^1(0,T;\mathcal{V}_h) \cap L^\infty(0,T;\mathcal{V}_h)$ with $u(0) = u_0$ and $v(0) = v_0$;

(b) *Irreversibility*: $t \mapsto v(t)$ is non-increasing (i.e., $v(s) \le v(t)$ a.e. in ω for every $0 \le t \le s \le T$) and $0 \le v(t) \le 1$ for every $t \in [0,T]$;

(c) *Displacement equilibrium*: for every $t \in [0,T]$ we have $u(t) = g(t)$ on $\partial\omega$ and

$$u(t) \in \arg\min\{\mathcal{E}_h(u, v(t)) : u \in \mathcal{U}_h \text{ with } u = g(t) \text{ on } \partial\omega\}\,;$$

(d) *Energy balance*: for a.e. $t \in [0,T]$ it holds

$$\dot{\mathcal{F}}_h(u(t), v(t)) = -\frac{1}{2}\|\dot{v}(t)\|^2_{\mathcal{V}_h} - \frac{1}{2}|\partial_v^- \mathcal{F}_h|^2_h(u(t), v(t)) + \mathcal{P}_h(u(t), v(t), \dot{g}(t))\,.$$

As we have done in Section 5.3, we immediately show that in order to obtain the balance (d) of Definition 5.4.9, only an energy inequality is sufficient. This is the content of Proposition 5.4.10, whose proof is similar to the one of Proposition 5.1.9.

Proposition 5.4.10. *Let $T > 0$, $h > 0$, $g \in AC([0,T];\mathcal{U}_h)$, $u_0 \in \mathcal{U}_h$, and $v_0 \in \mathcal{V}_h$ be such that* (5.53) *holds. Assume that the pair $(u, v)\colon [0,T] \to \mathcal{U}_h \times \mathcal{V}_h$ satisfies properties (a)–(d) of Definition 5.4.9 and that for every $t \in [0,T]$*

$$\mathcal{F}_h(u(t), v(t)) \le \mathcal{F}_h(u_0, v_0) - \frac{1}{2}\int_0^t |\partial_v^- \mathcal{F}_h|^2_{\mathcal{V}_h}(u(s), v(s)) + \|\dot{v}_h(s)\|^2_{\mathcal{V}_h}\,\mathrm{d}s + \int_0^t \mathcal{P}_h(u(s), v(s), \dot{g}(s))\,\mathrm{d}s\,.$$

Then, (u, v) also fulfills the energy balance (d) of Definition 5.4.9.

Finally, we conclude this subsection by providing a couple of general estimate regarding the discrete displacement field and the discrete phase field function. These results will be useful in the upcoming discussion of the finite-step algorithm.

Lemma 5.4.11. *Let $h > 0$. For $i = 1, 2$, let $g_i \in \mathcal{U}_h$ with $\|g_i\|_{H^1} \le M$, $v_i \in \mathcal{V}_h$ with $0 \le v_i \le 1$, and let*

$$u_i := \arg\min\{\mathcal{E}_h(u, v_i) : u \in \mathcal{U}_h, u = g_i \text{ on } \partial\omega\}\,.$$

Then, there exists $C_h > 0$, independent of g_i and v_i but depending on h, such that

$$\|u_1 - u_2\|_{H^1} \le C_h\|g_1 - g_2\|_{H^1} + C_h M\|v_1 - v_2\|_2\,.$$

Proof. We sketch the proof, which follows easily by Euler-Lagrange equations. Consider the auxiliary function $u_* := \arg\min\{\mathcal{E}_h(u, v_1) : u \in \mathcal{U}_h, u = g_2 \text{ on } \partial\omega\}$. We estimate

$\|u_1 - u_*\|_{H^1}$ and $\|u_* - u_2\|_{H^1}$. By continuous dependence with respect to the boundary data, it is easy to see that

$$\|u_1 - u_*\|_{H^1} \le C\|g_1 - g_2\|_{H^1} \,,$$

where $C > 0$ is actually independent of $h > 0$. By continuous dependence with respect to the coefficient it is also easy to see that

$$\|u_1 - u_*\|_{H^1} \le CM\|v_1 - v_2\|_{L^\infty} \le C_h M\|v_1 - v_2\|_{L^2} \,,$$

where the last inequality follows from the equivalence of norms in the finite dimensional space $\mathcal{V}_h$. $\square$

Lemma 5.4.12. *Let $h > 0$. For $i = 1, 2$, let $u_i \in \mathcal{U}_h$, $\bar{v} \in \mathcal{V}_h$ and let*

$$v_i \in \arg\min\Big\{\mathcal{F}_h(u_i, v) + \frac{1}{2\tau_k}\|v - \bar{v}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h\Big\} \,. \tag{5.54}$$

Then, there exists a constant $C_h > 0$, independent of u_i and $\bar{v}$ but depending on $h > 0$, such that

$$\|v_1 - v_2\|_{\mathcal{V}_h} \le \tau_k C_h\big(\|u_1\|_{H^1} + \|u_2\|_{H^1}\big)\|u_1 - u_2\|_{H^1} \,. \tag{5.55}$$

Proof. In view of (5.54), for $i = 1, 2$ the following equality holds:

$$\partial_v \mathcal{F}_h(u_i, v_i)[v_2 - v_1] + \frac{1}{\tau_k}\int_\omega \Pi_h\big((v_i - \bar{v})(v_2 - v_1)\big)\,\mathrm{d}x = 0 \,. \tag{5.56}$$

Subtracting the equality (5.56) for $i = 1$ to the one for $i = 2$, we obtain that

$$\big(\partial_v \mathcal{F}_h(u_2, v_2) - \partial_v \mathcal{F}_h(u_1, v_1)\big)[v_2 - v_1] + \frac{1}{\tau_k}\|v_2 - v_1\|^2_{\mathcal{V}_h} = 0 \,.$$

Adding and subtracting the term $\partial_v \mathcal{F}_h(u_1, v_2)[v_2 - v_1]$ and rearranging the terms, we deduce that

$$\begin{aligned}\frac{1}{\tau_k}\|v_2 - v_1\|^2_{\mathcal{V}_h} &+ \big(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_1, v_1)\big)[v_2 - v_1] \\ &= \big(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_2, v_2)\big)[v_2 - v_1] \,. \end{aligned} \tag{5.57}$$

The left-hand side of (5.57) can be simply estimated by

$$\frac{1}{\tau_k}\|v_2 - v_1\|^2_{\mathcal{V}_h} + \big(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_1, v_1)\big)[v_2 - v_1] \ge \frac{1}{\tau_k}\|v_2 - v_1\|^2_{\mathcal{V}_h} \,. \tag{5.58}$$

Indeed

$$\partial_v \mathcal{F}_h(u_1, v_2)[v_2 - v_1] = \int_\omega \Pi_h\big(v_2(v_2 - v_1)\big)\nabla u_1^\top A_1 \nabla u_1 \,\mathrm{d}x$$

$$+\int_\omega \nabla v_2^\top A_2 \nabla(v_2 - v_1)\,\mathrm{d}x + \Pi_h\big((v_2-1)(v_2-v_1)\big)h\,\mathrm{d}x\,.$$

and, similarly,

$$\begin{aligned}\partial_v \mathcal{F}_h(u_1, v_1)[v_2 - v_1] = &\int_\omega \Pi_h(v_1(v_2-v_1))\nabla u_1^\top A_1 \nabla u_1^\top\,\mathrm{d}x\\ &+\int_\omega \nabla v_1^\top A_2 \nabla(v_2 - v_1)\,\mathrm{d}x + \Pi_h\big((v_1-1)(v_2-v_1)\big)h\,\mathrm{d}x\,.\end{aligned}$$

Using the linearity of Π_h we easily get

$$\begin{aligned}\big(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_1, v_1)\big)[v_2 - v_1] = &\int_\omega \Pi_h\big((v_2-v_1)^2\big)\nabla u_1^\top A_1 \nabla u_1\,\mathrm{d}x\\ &+\int_\omega \nabla(v_2 - v_1)^\top A_2 \nabla(v_2 - v_1) \;+ \Pi_h\big((v_2-v_1)^2\big)h\,\mathrm{d}x \geq 0\,.\end{aligned}$$

As for the right-hand side of (5.57), we have that

$$\begin{aligned}&\big(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_2, v_2)\big)[v_2 - v_1]\\ &= \int_\omega \Pi_h\big(v_2(v_2-v_1)\big)\big(\nabla u_1^\top A_1 \nabla u_1 - \nabla u_2 A_1 \nabla u_2\big)\,\mathrm{d}x\\ &= \int_\omega \Pi_h\big(v_2(v_2-v_1)\big)\nabla(u_1+u_2)^\top A_1 \nabla(u_1-u_2)\,\mathrm{d}x\\ &\leq C\|\Pi_h(v_2(v_2-v_1))\|_{L^2}\|\nabla(u_1+u_2)\|_{L^\infty}\|\nabla(u_1-u_2)\|_{L^2}\,.\end{aligned} \tag{5.59}$$

where we used the symmetry of A_1. Abbreviate $w = \Pi_h(v_2(v_2 - v_1))$, then

$$w = \sum_{l=1}^{N_h}\Big(v_2(x_l)\big(v_2(x_l) - v_1(x_l)\big)\Big)\xi_l = \sum_{l=1}^{N_h} w(x_l)\xi_l\,.$$

Since $w \in \mathcal{V}_h$ we can use Lemma 5.4.2, hence $\|w\|_{L^2} \leq \|w\|_{\mathcal{V}_h}$. Note that

$$\|w\|^2_{\mathcal{V}_h} = \sum_{K\in\mathcal{T}_h}\int_K |\Pi_h(w^2)|\,\mathrm{d}x\,, \qquad \int_K |\Pi_h(w^2)|\,\mathrm{d}x = \sum_{i=1}^{3} w^2(x_i)\int_K \xi_i\,\mathrm{d}x\,,$$

where the points x_i are the vertices of the element K and the weights $\int_K \xi_i\,\mathrm{d}x$ are non-negative. By assumption $0 \leq v_2 \leq 1$, hence

$$\int_K |\Pi_h(w^2)|\,\mathrm{d}x \leq \sum_{i=1}^{3}\big(v_2(x_l) - v_1(x_l)\big)^2\int_K \xi_i\,\mathrm{d}x \;= \int_K \big|\Pi_h\big((v_2-v_1)^2\big)\big|\,\mathrm{d}x\,.$$

Taking the sum over all $K \in \mathcal{T}_h$ we get

$$\big\|\Pi_h\big(v_2(v_2-v_1)\big)\big\|^2_{\mathcal{V}_h} = \|w\|^2_{\mathcal{V}_h} \leq \|v_2 - v_1\|^2_{\mathcal{V}_h}\,.$$

Hence (5.59) yields

$$(\partial_v \mathcal{F}_h(u_1, v_2) - \partial_v \mathcal{F}_h(u_2, v_2))[v_2 - v_1] \\ \leq C\|v_2 - v_1\|_{\mathcal{V}_h} \|\nabla(u_1 + u_2)\|_{L^\infty} \|\nabla(u_1 - u_2)\|_{L^2} \,.$$

Combining the previous inequality with (5.57) – (5.58) yields

$$\frac{1}{\tau_k}\|v_1 - v_2\|_{\mathcal{V}_h} \leq C(\|u_1\|_{W^{1,\infty}} + \|u_2\|_{W^{1,\infty}})\|u_1 - u_2\|_{H^1} \,,$$

from which we get (5.55) by equivalence of norms in the finite dimensional space $\mathcal{U}_h$. The proof of the lemma is thus concluded. □

5.4.2 Multi-Step Algorithm

Let $T > 0$, $h > 0$, $g \in AC([0,T];\mathcal{U}_h)$, $u_0 \in \mathcal{U}_h$ and $v_0 \in \mathcal{V}_h$ with $u(0) = g(0)$ on $\partial\omega$ and $0 \leq v_0 \leq 1$ in ω. We now present the finite-step alternate minimization scheme (5.9)–(5.7), whose convergence is discussed in Theorems 5.4.14 and 5.4.18.

For every $k \in \mathbb{N}$ we define the time step $\tau_k := \frac{T}{k}$, and, for every $i \in \{0, \dots, k\}$, we set the discrete time nodes $t_i^k := i\tau_k$.

We construct recursively the displacement $u_i^k \in \mathcal{U}_h$ and the phase field functions $\tilde{v}_i^k, v_i^k \in \mathcal{V}_h$ at time t_i^k as follows: For $i = 0$ we set $u_0^k := u_0$ and $\tilde{v}_0^k = v_0^k := v_0$, while, for $i \geq 1$, we set $u_{i,0}^k := u_{i-1}^k$, $v_{i,0}^k := v_{i-1}^k$, and, for $j \geq 1$,

$$u_{i,j}^k := \arg\min\{\mathcal{E}_h(u, v_{i,j-1}^k) : u \in \mathcal{U}_h, u = g(t_i^k) \text{ on } \partial\omega\} \,, \tag{5.60}$$

$$\tilde{v}_{i,j}^k := \arg\min\left\{\mathcal{F}_h(u_{i,j}^k, v) + \frac{1}{2\tau_k}\|v - v_{i-1}^k\|_{\mathcal{V}_h}^2 : v \in \mathcal{V}_h\right\}. \tag{5.61}$$

As for $v_{i,j}^k$, we define it as the unique element of $\mathcal{V}_h$ satisfying

$$v_{i,j}^k(x_l) = \min\{\tilde{v}_{i,j}^k(x_l), v_{i-1}^k(x_l)\} \quad \text{for each vertex } x_l \in \Delta_h \,. \tag{5.62}$$

We notice that the minimum problems (5.60) and (5.61) admit unique solutions. We fix a priori an upper bound $J \geq 1$ on the number of steps of the algorithm. However, in order to take into account the cases in which the algorithm stops according to a certain criterion, as it is in the applications, we set

$$u_i^k := u_{i,J_i^k}^k \,, \qquad \tilde{v}_i^k := \tilde{v}_{i,J_i^k}^k \,, \qquad v_i^k := v_{i,J_i^k}^k \,, \tag{5.63}$$

where $1 \leq J_i^k \leq J$. Note that this setting includes any stopping criterion forcing an upper bound (arbitrarily large) on the number of iterations.

Remark 5.4.13. The algorithm described by (5.60)–(5.62) is a finite-dimensional adaptation inspired from the infinite-step scheme (5.2)–(5.3). In particular, the phase field minimum problem (5.61) is unconstrained, while the irreversibility is taken into account in (5.62), where the constraint is imposed only in the nodes of the triangulation $\mathcal{T}_h$; note indeed that the function $\min\{\tilde{v}_{i,j}^k, v_{i-1}^k\}$ (where the minimum is pointwise in ω) in general does not belong to $\mathcal{V}_h$.

As in Sections 5.3, we define for all $t \in [t_i^k, t_{i+1}^k)$ the interpolation functions

$$v_k(t) := v_i^k + \frac{v_{i+1}^k - v_i^k}{\tau_k}(t - t_i^k)\,, \quad \underline{u}_k(t) := u_i^k\,, \quad \underline{v}_k(t) := v_i^k\,, \tag{5.64}$$

and for all $t \in [t_{i-1}^k, t_i^k)$

$$\bar{u}_k(t) := u_i^k\,, \quad \bar{v}_k(t) := v_i^k\,, \quad \tilde{v}_k(t) := \tilde{v}_i^k\,, \quad t_k(t) := t_i^k\,. \tag{5.65}$$

The convergence result obtained in this subsection is the subject of the following theorem.

Theorem 5.4.14. *There exists a subsequence, not relabelled, of the pair* $(\bar{u}_k, v_k)$ *such that:*

(a) $v_k \rightharpoonup v$ *in* $H^1([0,T]; \mathcal{V}_h)$*;*

(b) $v_k(t) \to v(t)$ *in* $\mathcal{V}_h$ *and* $\bar{u}_k(t) \to u(t)$ *in* $\mathcal{U}_h$ *for every* $t \in [0,T]$*;*

(c) (u, v) *is a finite-dimensional unilateral* L^2*-gradient flow for* $\mathcal{F}$*, in the sense of Definition 5.4.9.*

The rest of this subsection is devoted to the proof of Theorem 5.4.14. We start by showing some properties of the functions defined in (5.61) and (5.62).

Proposition 5.4.15. *Let* $\tilde{v}_{i,j}^k$ *and* $v_{i,j}^k$ *be as in* (5.61) *and* (5.62)*, respectively. Then* $0 \le v_{i,j}^k, \tilde{v}_{i,j}^k \le 1$ *in* ω*.*

Proof. In view of (5.62), it is enough to prove $0 \le \tilde{v}_{i,j}^k \le 1$ on ω assuming that $0 \le v_{i-1}^k \le 1$ (remember that we assume $0 \le v_0 \le 1$ in ω). By contradiction, let us first suppose that $\tilde{v}_{i,j}^k \not\ge 0$. Let $x_l \in \Delta_h$ be such that $\tilde{v}_{i,j}^k(x_l) \le \tilde{v}_{i,j}^k(x_m)$ for every $m = 1, \dots, N_h$. In particular, we have $\tilde{v}_{i,j}^k(x_l) < 0$. Let $\xi_l \ge 0$ be the l-th element of the basis of $\mathcal{V}_h$ defined by (5.50). By (5.61), we deduce that

$$\begin{aligned} 0 = \partial_v \mathcal{F}_h(u_{i,j}^k, \tilde{v}_{i,j}^k)[\xi_l] &= \int_\omega \Pi_h(\tilde{v}_{i,j}^k \xi_l)\big(\nabla u_{i,j}^k\big)^\top A_1 \nabla u_{i,j}^k \,\mathrm{d}x + \int_\omega \big(\nabla \tilde{v}_{i,j}^k\big)^\top A_2 \nabla \xi_l \,\mathrm{d}x \\ &\quad - \int_\omega \Pi_h\big((1 - \tilde{v}_{i,j}^k)\xi_l\big) h \,\mathrm{d}x + \frac{1}{\tau_k}\int_\omega \Pi_h\big((\tilde{v}_{i,j}^k - v_{i-1}^k)\xi_l\big) \,,\mathrm{d}x\,. \end{aligned} \tag{5.66}$$

Since $\tilde{v}_{i,j}^k(x_l) < 0$ and $\xi_l(x_m) = \delta_{ml}$, we have

$$\Pi_h(\tilde{v}_{i,j}^k \xi_l) = \sum_{m=1}^{N_h} \big(\tilde{v}_{i,j}^k(x_m)\xi_l(x_m)\big)\xi_m = \tilde{v}_{i,j}^k(x_l)\xi_l \le 0\,, \quad \Pi_h\big((\tilde{v}_{i,j}^k - v_{i-1}^k)\xi_l\big) \le 0$$

$$\Pi_h\big((1 - \tilde{v}_{i,j}^k)\xi_l\big) = \big(1 - \tilde{v}_{i,j}^k(x_l)\big)\xi_l \ge 0\,, \quad \text{with} \int_\omega \Pi_h\big((1 - \tilde{v}_{i,j}^k)\xi_l\big)\,\mathrm{d}x > 0\,.$$

Hence, from (5.66) we get

$$\int_\omega (\nabla \tilde{v}^k_{i,j})^\top A_2 \nabla \xi_l \,\mathrm{d}x = -\int_\omega \Pi_h(\tilde{v}^k_{i,j}\xi_l)(\nabla u^k_{i,j})^\top A_1 \nabla u^k_{i,j}\,\mathrm{d}x \\ + \int_\omega \Pi_h((1-\tilde{v}^k_{i,j})\xi_l)h\,\mathrm{d}x - \frac{1}{\tau_k}\int_\omega \Pi_h((\tilde{v}^k_{i,j} - v^k_{i-1})\xi_l)\,\mathrm{d}x > 0\,. \tag{5.67}$$

On the other hand, writing $\tilde{v}^k_{i,j} = \sum_{m=1}^{N_h} \tilde{v}^k_{i,j}(x_m)\xi_m$, by direct computation we get

$$\begin{aligned} &\int_\omega (\nabla \tilde{v}^k_{i,j})^\top A_2 \nabla \xi_l \,\mathrm{d}x \\ &= \sum_{m=1}^{N_h} \tilde{v}^k_{i,j}(x_m)\int_\omega \nabla\xi_m^\top A_2 \nabla\xi_l\,\mathrm{d}x \\ &= \tilde{v}^k_{i,j}(x_l)\sum_{m=1}^{N_h}\int_\omega \nabla\xi_m^\top A_2\nabla\xi_l\,\mathrm{d}x + \sum_{m=1}^{N_h}(\tilde{v}^k_{i,j}(x_m) - \tilde{v}^k_{i,j}(x_l))\int_\omega \nabla\xi_m^\top A_2\nabla\xi_l\,\mathrm{d}x \\ &= \sum_{m=1}^{N_h}(\tilde{v}^k_{i,j}(x_m) - \tilde{v}^k_{i,j}(x_l))\int_\omega \nabla\xi_m^\top A_2\nabla\xi_l\,\mathrm{d}x \le 0\,, \end{aligned} \tag{5.68}$$

where, in the last equality, we have used (5.51), the fact that $\tilde{v}^k_{i,j}(x_l) \le \tilde{v}^k_{i,j}(x_m)$ for every $m = 1,\dots,N_h$, and

$$\sum_{m=1}^{N_h}\int_\omega \nabla\xi_m^\top A_2\nabla\xi_l\,\mathrm{d}x = \int_\omega \nabla\mathbb{1}^\top A_2\nabla\xi_l\,\mathrm{d}x = 0\,.$$

Therefore, combining (5.67) and (5.68) we get a contradiction, and thus $\tilde{v}^k_{i,j} \ge 0$.

With a similar argument, we can also show that $\tilde{v}^k_{i,j} \le 1$. □

The following proposition is the discrete counterpart of Proposition 5.3.2 for the discrete unilateral L^2-slope $|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}$.

Proposition 5.4.16. *Let $h > 0$, $k \in \mathbb{N}\setminus\{0\}$, u^k_i, $\tilde{v}^k_i$, and v^k_i be defined as in* (5.60)-(5.63)*, for every $i \in \{1,\dots,k\}$. Then*

$$\frac{\|v^k_i - v^k_{i-1}\|_{\mathcal{V}_h}}{\tau_k} = |\partial_v^-\mathcal{F}_h|_{\mathcal{V}_h}(u^k_i,\tilde{v}^k_i)\,, \tag{5.69}$$

$$\partial_v\mathcal{F}_h(u^k_i,\tilde{v}^k_i)[v^k_i - v^k_{i-1}] = -|\partial_v^-\mathcal{F}_h|_{\mathcal{V}_h}(u^k_i,\tilde{v}^k_i)\|v^k_i - v^k_{i-1}\|_{\mathcal{V}_h}\,, \tag{5.70}$$

$$\partial_v\mathcal{F}_h(u^k_i,v^k_i)[v^k_i - v^k_{i-1}] \le \partial_v\mathcal{F}_h(u^k_i,\tilde{v}^k_i)[v^k_i - v^k_{i-1}]\,. \tag{5.71}$$

Note that in the continuum setting the counterpart of (5.71) holds with an identity.

Proof. Let us start with (5.69). In view of the definition of $\tilde{v}^k_i$, for every $\varphi \in \mathcal{V}_h$ it holds

$$\partial_v\mathcal{F}_h(u^k_i,\tilde{v}^k_i)[\varphi] + \frac{1}{\tau_k}\int_\omega \Pi_h((\tilde{v}^k_i - v^k_{i-1})\varphi)\,\mathrm{d}x = 0\,.$$

Therefore,

$$\begin{aligned}|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_i^k, \tilde{v}_i^k) &= \sup\{-\partial_v \mathcal{F}_h(u_i^k, \tilde{v}_i^k)[\varphi] : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1\} \\ &= \sup\left\{\frac{1}{\tau_k}\int_\omega \Pi_h\big((\tilde{v}_i^k - v_{i-1}^k)\varphi\big)\,\mathrm{d}x : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1\right\}.\end{aligned} \tag{5.72}$$

In order to obtain (5.69) and (5.70), we will show that the supremum in the right-hand side of (5.72) is attained for $\varphi = \frac{v_i^k - v_{i-1}^k}{\|v_i^k - v_{i-1}^k\|_{\mathcal{V}_h}}$. By definition of Π_h we can write

$$\int_\omega \Pi_h\big((\tilde{v}_i^k - v_{i-1}^k)\varphi\big)\,\mathrm{d}x = \sum_{l=1}^{N_h} (\tilde{v}_i^k(x_l) - v_{i-1}^k(x_l))\varphi(x_l)\int_\omega \xi_l\,\mathrm{d}x .$$

Hence, being $\varphi \leq 0$, we can rewrite (5.72) as

$$\begin{aligned}|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_i^k, \tilde{v}_i^k) = \sup\Big\{\frac{1}{\tau_k}\int_\omega \Pi_h\big((\tilde{v}_i^k - v_{i-1}^k)\varphi\big)\,\mathrm{d}x : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1, \\ \varphi(x_l) = 0 \text{ if } x_l \in \Delta_h \text{ and } \tilde{v}_i^k(x_l) - v_{i-1}^k(x_l) > 0\Big\}.\end{aligned} \tag{5.73}$$

Remember that $v_i^k(x_l) = \min\{\tilde{v}_i^k(x_l), v_{i-1}^k(x_l)\}$ in each vertex $x_l \in \Delta_h$. Hence, for every $\varphi \in \mathcal{V}_h$ satisfying the constraints in (5.73) we have

$$\Pi_h\big((\tilde{v}_i^k - v_{i-1}^k)\varphi\big) = \Pi_h\big((v_i^k - v_{i-1}^k)\varphi\big) , \tag{5.74}$$

which implies, together with (5.73),

$$\begin{aligned}|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_i^k, \tilde{v}_i^k) = \sup\Big\{\frac{1}{\tau_k}\int_\omega \Pi_h\big((v_i^k - v_{i-1}^k)\varphi\big)\,\mathrm{d}x : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1, \\ \varphi(x_l) = 0 \text{ if } x_l \in \Delta_h \text{ and } \tilde{v}_i^k(x_l) - v_{i-1}^k(x_l) > 0\Big\}.\end{aligned} \tag{5.75}$$

By (5.62) and (5.63) we know that $v_i^k(x_l) = v_{i-1}^k(x_l)$ for every vertex $x_l \in \Delta_h$ such that $\tilde{v}_i^k(x_l) - v_{i-1}^k(x_l) > 0$. Thus, equality (5.75) can be rewritten in the simpler form

$$|\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_i^k, \tilde{v}_i^k) = \sup\left\{\frac{1}{\tau_k}\int_\omega \Pi_h\big((v_i^k - v_{i-1}^k)\varphi\big)\,\mathrm{d}x : \varphi \in \mathcal{V}_h, \varphi \leq 0, \|\varphi\|_{\mathcal{V}_h} \leq 1\right\}. \tag{5.76}$$

It is then easy to see that the supremum in (5.76) is actually attained for $\varphi = -\frac{v_i^k - v_{i-1}^k}{\|v_i^k - v_{i-1}^k\|_{\mathcal{V}_h}}$.

In order to prove (5.71), we need to estimate each term of

$$\partial_v \mathcal{F}_h(u_i^k, \tilde{v}_i^k)[v_i^k - v_{i-1}^k] = I_1 + I_2 + I_3 , \tag{5.77}$$

with

$$
\begin{aligned}
I_1 &:= \int_\omega \Pi_h\big(\tilde{v}_i^k(v_i^k - v_{i-1}^k)\big)(\nabla u_i^k)^\top A_1 \nabla u_i^k \,\mathrm{d}x \\
I_2 &:= \int_\omega (\nabla \tilde{v}_i^k)^\top A_2 \nabla (v_i^k - v_{i-1}^k)\,\mathrm{d}x \\
I_3 &:= -\int_\omega \Pi_h\big((1-\tilde{v}_i^k)(v_i^k - v_{i-1}^k)\big) h \,\mathrm{d}x\,.
\end{aligned}
$$

Let us start with I_1. By the same argument used in (5.74), we have that

$$
\Pi_h\big(\tilde{v}_i^k(v_i^k - v_{i-1}^k)\big) = \Pi_h\big(v_i^k(v_i^k - v_{i-1}^k)\big)\,,
$$

so that

$$
I_1 = \int_\omega \Pi_h\big(v_i^k(v_i^k - v_{i-1}^k)\big)(\nabla u_i^k)^\top A_1 \nabla u_i^k \,\mathrm{d}x\,. \tag{5.78}
$$

In a similar way, we can also show that

$$
I_3 = -\int_\omega \Pi_h\big((1-v_i^k)(v_i^k - v_{i-1}^k)\big) h \,\mathrm{d}x\,. \tag{5.79}
$$

As for I_2, we write the scalar product in terms of the basis $\{\xi_l\}_{l=1}^{N_h}$ of $\mathcal{V}_h$. Thus,

$$
\begin{aligned}
I_2 = {} & \sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big) \sum_{l=1}^{N_h} \tilde{v}_i^k(x_l) \int_\omega (\nabla \xi_l)^\top A_2 \nabla \xi_m \,\mathrm{d}x \\
= {} & \sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big)\tilde{v}_i^k(x_m) \int_\omega (\nabla \xi_m)^\top A_2 \nabla \xi_m \,\mathrm{d}x \\
& + \sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big) \sum_{\substack{l=1\\ l\neq m}}^{N_h} \tilde{v}_i^k(x_l) \int_\omega (\nabla \xi_l)^\top A_2 \nabla \xi_m \,\mathrm{d}x\,.
\end{aligned}
$$

By construction we have that $v_i^k \le \tilde{v}_i^k$ and $v_i^k \le v_{i-1}^k$. Therefore, by (5.51) we easily get

$$
\begin{aligned}
& \sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big) \sum_{\substack{l=1\\ l\neq m}}^{N_h} \tilde{v}_i^k(x_l) \int_\omega (\nabla \xi_l)^\top A_2 \nabla \xi_m \mathrm{d}x \\
& \qquad \ge \sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big) \sum_{\substack{l=1\\ l\neq m}}^{N_h} v_i^k(x_l) \int_\omega (\nabla \xi_l)^\top A_2 \nabla \xi_m \mathrm{d}x\,.
\end{aligned}
$$

Moreover, arguing as in (5.74), we deduce that

$$
\sum_{m=1}^{N_h} \big(v_i^k(x_m) - v_{i-1}^k(x_m)\big)\tilde{v}_i^k(x_m) \int_\omega (\nabla \xi_m)^\top A_2 \nabla \xi_m \,\mathrm{d}x
$$

$$= \sum_{m=1}^{N_h} (v_i^k(x_m) - v_{i-1}^k(x_m)) v_i^k(x_m) \int_\omega (\nabla \xi_m)^\top A_2 \nabla \xi_m \, \mathrm{d}x \,.$$

Hence, we obtain

$$I_2 \geq \int_\omega (\nabla v_i^k)^\top A_2 \nabla (v_i^k - v_{i-1}^k) \, \mathrm{d}x \,. \tag{5.80}$$

Finally, inserting (5.78), (5.79) and (5.80) in (5.77) implies

$$\begin{aligned}
&\partial_v \mathcal{F}_h(u_i^k, \tilde{v}_i^k)[v_i^k - v_{i-1}^k] \\
&\geq \int_\omega \Pi_h(v_i^k(v_i^k - v_{i-1}^k))(\nabla u_i^k)^\top A_1 \nabla u_i^k \, \mathrm{d}x \\
&\quad + \int_\omega (\nabla v_i^k)^\top A_2 \nabla (v_i^k - v_{i-1}^k) \, \mathrm{d}x - \int_\omega \Pi_h\big((1 - v_i^k)(v_i^k - v_{i-1}^k)\big) h \, \mathrm{d}x \\
&= \partial_v \mathcal{F}_h(u_i^k, v_i^k)[v_i^k - v_{i-1}^k] \,,
\end{aligned}$$

which is exactly (5.71). This concludes the proof of the proposition. □

In the following proposition, we obtain the finite-dimensional counterpart of the energy inequality (5.44), as well as some uniform bounds for the sequences (5.64)–(5.65).

Proposition 5.4.17. *Let $h > 0$. Then, the following facts hold:*

(a) The sequence v_k is bounded in $L^\infty([0,T]; \mathcal{V}_h)$ and in $H^1([0,T]; \mathcal{V}_h)$;

(b) The sequences $\bar{v}_k$, $\tilde{v}_k$, $\underline{v}_k$ are bounded in $L^\infty([0,T]; H^1(\omega))$;

(c) The sequences $\bar{u}_k$ and $\underline{u}_k$ are bounded in $L^\infty([0,T]; \mathcal{U}_h)$;

(d) There exists $R_k \to 0^+$ as $k \to +\infty$ such that for every $t \in [0,T]$ it holds

$$\begin{aligned}
\mathcal{F}_h(\bar{u}_k(t), \bar{v}_k(t)) \leq \mathcal{F}_h(u_0, v_0) - \frac{1}{2} \int_0^{t_k(t)} \|\dot{v}_k(s)\|_{\mathcal{V}_h}^2 + |\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}^2 (\bar{u}_k(s), \tilde{v}_k(s)) \, \mathrm{d}s \\
+ \int_0^{t_k(t)} \mathcal{P}_h(\underline{u}_k(s), \underline{v}_k(s), \dot{g}(s)) \, \mathrm{d}s + R_k \,.
\end{aligned} \tag{5.81}$$

In particular the energy $\mathcal{F}_h(\bar{u}_k(t), \bar{v}_k(t))$ is uniformly bounded, w.r.t. t and k.

Proof. The argument used to prove this proposition is similar to the one presented in Propositions 5.3.4. We show here where to apply the estimates shown in Lemmas 5.4.11 and 5.4.12 and in Proposition 5.4.16.

Let us fix $k \in \mathbb{N} \setminus \{0\}$, $i \in \{1, \dots, k\}$, and $t \in (t_{i-1}^k, t_i^k]$. By convexity of $\mathcal{F}_h(u_i^k, \cdot)$, we have

$$\mathcal{F}_h(u_i^k, v_{i-1}^k) \geq \mathcal{F}_h(u_i^k, v_i^k) + \partial_v \mathcal{F}_h(u_i^k, v_i^k)[v_{i-1}^k - v_i^k] \,.$$

In view of (5.71), we can continue with

$$\mathcal{F}_h(u_i^k, v_{i-1}^k) \geq \mathcal{F}_h(u_i^k, v_i^k) + \partial_v \mathcal{F}_h(u_i^k, \tilde{v}_i^k)[v_{i-1}^k - v_i^k] \,.$$

Taking into account (5.69) and (5.70), we deduce that

$$\mathcal{F}_h(u_i^k, v_{i-1}^k) \geq \mathcal{F}_h(u_i^k, v_i^k) + \frac{1}{2}\int_{t_{i-1}^k}^{t_i^k} \|\dot{v}_k^h(s)\|^2_{\mathcal{V}_h} + |\partial_v^- \mathcal{F}_h|^2_{\mathcal{V}_h}(\bar{u}_k(s), \tilde{v}_k(s))\,\mathrm{d}s\,. \tag{5.82}$$

In order to pass from u_i^k to u_{i-1}^k in the left-hand side of (5.82), we first make an intermediate step exploiting the construction of $u_{i,1}^k$ in the multi-step algorithm. Exploiting again the quadratic structure of the functional $\mathcal{F}_h$ and the stability of $u_{i,1}^k$, and recalling that $u_i^k = u_{i,1}^k = g(t_i^k)$ on $\partial\Omega$, we have that

$$\begin{aligned} \mathcal{F}_h(u_i^k, v_{i-1}^k) &= \mathcal{F}_h(u_{i,1}^k + (u_i^k - u_{i,1}^k), v_{i-1}^k) \\ &= \mathcal{F}_h(u_{i,1}^k, v_{i-1}^k) + \mathcal{E}_h(u_i^k - u_{i,1}^k, v_{i-1}^k) \\ &\quad + \int_\Omega ((v_{i-1}^k)^2 + \eta)\nabla(u_{i,1}^k)^\top A_1 \nabla(u_i^k - u_{i,1}^k)\,\mathrm{d}x \\ &= \mathcal{F}_h(u_{i,1}^k, v_{i-1}^k) + \mathcal{E}_h(u_i^k - u_{i,1}^k, v_{i-1}^k)\,. \end{aligned} \tag{5.83}$$

Since v_{i-1}^k takes values in the interval $[0,1]$ and A_1 is positive definite, in view of (5.83) there exists a positive constant C such that

$$\mathcal{F}_h(u_i^k, v_{i-1}^k) \leq \mathcal{F}_h(u_{i,1}^k, v_{i-1}^k) + C\|u_i^k - u_{i,1}^k\|^2_{H^1}\,. \tag{5.84}$$

As we argued in (5.47) and (5.48), by the minimality of $u_{i,1}^k$ and the regularity of the boundary datum g, we can continue in (5.84) with

$$\begin{aligned} \mathcal{F}_h(u_i^k, v_{i-1}^k) \leq \mathcal{F}_h(u_{i-1}^k, v_{i-1}^k) &+ \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}_h(\bar{u}_k(s), \underline{v}_k(s), \dot{g}(s))\,\mathrm{d}s \\ &+ C\|g(t_i^k) - g(t_{i-1}^k)\|^2_{H^1} + C\|u_i^k - u_{i,1}^k\|^2_{H^1}\,, \end{aligned}$$

for some constant $C > 0$ depending only on the matrix A_1. Thanks to Lemma 5.4.11, the previous inequality becomes

$$\begin{aligned} \mathcal{F}_h(u_i^k, v_{i-1}^k) \leq \mathcal{F}_h(u_{i-1}^k, v_{i-1}^k) &+ \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}_h(\bar{u}_k^h(s), \underline{v}_k^h(s), \dot{g}(s))\,\mathrm{d}s \\ &+ C\|g(t_i^k) - g(t_{i-1}^k)\|^2_{H^1} + C\|v_{i,J_i^k-1}^k - v_{i-1}^k\|^2_{\mathcal{V}_h}\,. \end{aligned}$$

If $J_i^k \geq 2$ we write

$$\begin{aligned} \mathcal{F}_h(u_i^k, v_{i-1}^k) \leq \mathcal{F}_h(u_{i-1}^k, v_{i-1}^k) &+ \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}_h(\bar{u}_k^h(s), \underline{v}_k^h(s), \dot{g}(s))\,\mathrm{d}s \\ &+ C\|g(t_i^k) - g(t_{i-1}^k)\|^2_{H^1} + C\|v_i^k - v_{i,J_i^k-1}^k\|^2_{\mathcal{V}_h} + C\|v_i^k - v_{i-1}^k\|^2_{\mathcal{V}_h}\,. \end{aligned}$$

Applying Lemma 5.4.12 to u_i^k, u^k_{i,J_i^k-1} and $\bar v = v^k_{i-1}$ we deduce that

$$\|v_i^k - v^k_{i,J_i^k-1}\|_{\mathcal{V}_h} \leq \|\tilde v_i^k - \tilde v^k_{i,J_i^k-1}\|_{\mathcal{V}_h} \leq C_h \tau_k (\|u_i^k\|_{H^1} + \|u^k_{i,J_i^k-1}\|_{H^1}) \|u_i^k - u^k_{i,J_i^k-1}\|_{H^1} \,.$$

Note that by minimality there holds

$$\mathcal{E}_h(u_i^k, v^k_{i,J_i^k-1}) \leq C(1+\eta)\|g_i^k\|_{H^1} \quad \text{and} \quad \mathcal{E}_h(u^k_{i,J_i^k-1}, v^k_{i,J_i^k-2}) \leq C(1+\eta)\|g_i^k\|_{H^1} \,.$$

Since g_i^k is bounded in H^1 uniformly with respect to i and k, and A_1 is positive definite we get $\|u_i^k\|_{H^1} + \|u^k_{i,J_i^k-1}\|_{H^1}$ is bounded uniformly with respect to i and k; hence

$$\|v_i^k - v^k_{i,J_i^k-1}\|_{\mathcal{V}_h} \leq C_h \tau_k \,,$$

for some positive constant C_h independent of i and k. Then, for every $J_i^k \geq 1$ we obtain

$$\mathcal{F}_h(u_i^k, v_{i-1}^k) \leq \mathcal{F}_h(u_{i-1}^k, v_{i-1}^k) + \int_{t_{i-1}^k}^{t_i^k} \mathcal{P}_h(\bar u_k^h(s), \underline{v}_k^h(s), \dot g(s))\,\mathrm{d}s + \\ C\big\|g(t_i^k) - g(t_{i-1}^k)\big\|^2_{H^1} + C_h\tau_k^2 + C\|v_i^k - v_{i-1}^k\|^2_{\mathcal{V}_h} \,. \quad (5.85)$$

Combining inequalities (5.82) and (5.85) and iterating over i, we get the estimate

$$\begin{aligned} &\mathcal{F}_h(\bar u_k(t), \bar v_k(t)) + \frac{1}{2}\int_0^{t_k(t)} \big\|\dot v_k(s)\big\|^2_{\mathcal{V}_h} + |\partial_v^- \mathcal{F}_h|^2_{\mathcal{V}_h}(\bar u_k(s), \tilde v_k(s))\,\mathrm{d}s \\ &\leq \mathcal{F}_h(u_0, v_0) + \int_0^{t_k(t)} \mathcal{P}_h(\underline{u}_k^h(s), \underline{v}_k^h(s), \dot g(s))\,\mathrm{d}s \\ &\quad + C\sum_{i=1}^I \big\|g(t_i^k) - g(t_{i-1}^k)\big\|^2_{H^1} + C\tau_k T + C\sum_{i=1}^I \|v_i^k - v_{i-1}^k\|^2_{\mathcal{V}_h} \,, \end{aligned} \quad (5.86)$$

where $I \in \{1, \ldots, k\}$ is such that $t_k(t) = t_I^k$.

In order to proceed in the estimate (5.86), we notice that

$$\sum_{j=1}^I \|v_j^k - v_{j-1}^k\|^2_{\mathcal{V}_h} = \tau_k \int_0^{t_k(t)} \|\dot v_k(s)\|^2_{\mathcal{V}_h}\,\mathrm{d}s \,. \quad (5.87)$$

Combining (5.86) and (5.87), we deduce that for k large enough it holds

$$\begin{aligned} &\mathcal{F}_h(\bar u_k(t), \bar v_k(t)) + \frac{1}{4}\int_0^{t_k(t)} \big\|\dot v_k(s)\big\|^2_{L^2}\,\mathrm{d}s \\ &\quad \leq \mathcal{F}_h(u_0, v_0) + \int_0^{t_k(t)} \mathcal{P}_h(\underline{u}_k(s), \underline{v}_k(s), \dot g(s))\,\mathrm{d}s + C'\sum_{j=1}^I \big\|g(t_j^k) - g(t_{j-1}^k)\big\|^2_{H^1} \,, \end{aligned}$$

Following the argument of the proof of Proposition 5.3.4, we obtain that u_k, $\bar{u}_k$, and $\underline{u}_k$ are bounded in $L^\infty([0,T];\mathcal{U}_h)$, v_k is bounded in $H^1([0,T];\mathcal{V}_h)$, and v_k, $\tilde{v}_k$, $\bar{v}_k$, and $\underline{v}_k$ are bounded in $L^\infty([0,T];H^1(\omega))$. To conclude, it is enough to define

$$R_k := C\sum_{i=1}^{k}\big\|g(t_i^k) - g(t_{i-1}^k)\big\|_{H^1}^2 + C\tau_k T + C\sum_{i=1}^{k}\big\|v_i^k - v_{i-1}^k\big\|_{\mathcal{V}_h}^2 .$$

By the regularity of the boundary datum $g \in AC([0,T];\mathcal{U}_h)$ and the boundedness of v_k in $H^1([0,T];\mathcal{V}_h)$, we get that $R_k \to 0$ as $k \to +\infty$. □

We are now in a position to prove Theorem 5.4.14, performing the passage to the time-continuous limit of the sequences of interpolation functions defined in (5.64)–(5.65).

Proof of Theorem 5.4.14. In view of the bounds (a) and (b) in Proposition 5.4.17, there exists a function $v \in H^1([0,T];\mathcal{V}_h)$ such that, up to a subsequence, $v_k \rightharpoonup v$ weakly in $H^1([0,T];\mathcal{V}_h)$. This implies that $v_k(t) \to v(t)$ in $\mathcal{V}_h$ for every $t \in [0,T]$ and that $v \in L^\infty([0,T];\mathcal{V}_h)$ (remember that in the finite-dimensional setting weak and strong topologies are equivalent). It is also easy to see that v satisfies the irreversibility condition (b) of Definition 5.4.9. Since, by construction,

$$\big\|\underline{v}_k(t) - v_k(t)\big\|_{\mathcal{V}_h} \le \tau_k^{1/2}\bigg(\int_0^T \big\|\dot{v}_k(s)\big\|_{\mathcal{V}_h}^2\,\mathrm{d}s\bigg)^{1/2} \quad \text{for all } t \in [0,T]\,,$$

we have that $\underline{v}_k(t) \to v(t)$ in $\mathcal{V}_h$ for $t \in [0,T]$. In a similar way, we also get that $\bar{v}_k(t) \to v(t)$ in $\mathcal{V}_h$ for every $t \in [0,T]$. Moreover, by (5.61) and by Proposition 5.4.17, we get

$$\big\|\tilde{v}_k(t) - \underline{v}_k(t)\big\|_{\mathcal{V}_h}^2 \le 2\tau_k\,\mathcal{F}_h(\bar{u}_k(t), \underline{v}_k(t)) \le C\tau_k\,,$$

for some positive constant C independent of k. Therefore, $\tilde{v}_k(t) \to v(t)$ in $\mathcal{V}_h$ for every $t \in [0,T]$.

As for the sequences $\bar{u}_k$ and $\underline{u}_k$, by (c) of Proposition 5.4.17 we have that for every $t \in [0,T]$ there exists $u(t) \in \mathcal{U}_h$ such that, up to a subsequence, $\bar{u}_k(t) \to u(t)$ in $\mathcal{U}_h$. Applying [2, Lemma 3.2], we can prove that the converging subsequence does not depend on $t \in [0,T]$, that $\underline{u}_k(t) \to u(t)$ in $\mathcal{U}_h$ for every $t \in [0,T]$, and that the pair $\big(u(t), v(t)\big)$ satisfies the displacement equilibrium condition (c) of Definition 5.4.9.

Since $v \in H^1([0,T];\mathcal{V}_h)$, by continuous dependence for the displacement, see Lemma 5.4.11, we easily deduce the time regularity of u, that is, $u \in C([0,T];\mathcal{U}_h)$.

It remains to prove the energy balance (d) of Definition 5.4.9. Applying (a) of Lemma 5.4.8 and Fatou's Lemma, we can pass to the lim inf as $k \to +\infty$ in the energy estimate (5.81), obtaining the inequality

$$\begin{aligned}\mathcal{F}_h\big(u(t), v(t)\big) \le \mathcal{F}_h\big(u(0), v(0)\big) - \frac{1}{2}\int_0^t \big\|\dot{v}_h(s)\big\|_{\mathcal{V}_h}^2 + |\partial_v^- \mathcal{F}_h|_h^2(u(s), v(s))\,\mathrm{d}s \\ + \int_0^t \mathcal{P}_h(u(s), v(s), \dot{g}(s))\,\mathrm{d}s\,.\end{aligned}$$

The opposite inequality follows from Proposition 5.4.10. □

5.4.3 Convergence to the continuum

We conclude this chapter by showing that any limit of a sequence of finite-dimensional unilateral L^2-gradient flow taken as the mesh becomes finer and finer (i.e., as $h \to 0$) is itself a unilateral L^2-gradient flow. This is the content of the following theorem.

Theorem 5.4.18. *Let $T > 0$, $g \in AC([0,T]; W^{1,p}(\omega;\mathbb{R}^2))$, $v_0 \in H^1(\omega)$ with $0 \le v_0 \le 1$, and*

$$u_0 \in \arg\min\{\mathcal{E}(u, v_0) : u \in \mathcal{U}, u = g(0) \text{ on } \partial\omega\}\,.$$

Assume that there exist the sequences $v_{0,h} \in \mathcal{V}_h$ and $g_h \in AC([0,T];\mathcal{U}_h)$ such that $0 \le v_{0,h} \le 1$, $v_{0,h} \to v_0$ in $H^1(\omega)$ and $g_h \to g$ in $W^{1,1}([0,T];\mathcal{U})$, as $h \to 0$. Let

$$u_{0,h} \in \arg\min\{\mathcal{E}_h(u, v_0) : u \in \mathcal{U}_h, u = g_h(0) \text{ on } \partial\omega\}\,.$$

For every $h > 0$, let $(u_h, v_h)\colon [0,T] \to \mathcal{U}_h \times \mathcal{V}_h$ be a finite-dimensional unilateral L^2-gradient flow for the energy $\mathcal{F}_h$ with initial conditions $(u_{0,h}, v_{0,h})$ and boundary condition g_h.

Then, there exists a unilateral L^2-gradient flow $(u, v)\colon [0,T] \to \mathcal{U} \times \mathcal{V}$ with initial conditions (u_0, v_0) and boundary conditions g such that, up to a subsequence independent of $t \in [0,T]$, $u_h(t) \to u(t)$ in $\mathcal{U}$ and $v_h(t) \rightharpoonup v(t)$ weakly in $H^1(\omega)$.

In order to prove Theorem 5.4.18, we first need to show a lower semi-continuity property of the energy and of the unilateral slope, when passing from the space-discrete to the space-continuous setting.

Lemma 5.4.19. *Let $u_h \in \mathcal{U}_h$, $v_h \in \mathcal{V}_h$, $u \in \mathcal{U}$ and $v \in \mathcal{V}$ with $0 \le v_h, v \le 1$. If $u_h \to u$ in $\mathcal{U}$ and $v_h \rightharpoonup v$ weakly in $H^1(\omega)$, then*

$$\mathcal{F}(u,v) \le \liminf_{h\to 0} \mathcal{F}_h(u_h, v_h) \quad \text{and} \quad |\partial_v^- \mathcal{F}|(u,v) \le \liminf_{h\to 0} |\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_h, v_h)\,.$$

Proof. As a preliminary step, let us show that $\Pi_h(v_h^2) \to v^2$ in $L^1(\omega)$. By classical interpolation estimates, e.g., [46, Theorem 3.1.6], for every element $K \in \mathcal{T}_h$ we have

$$\|\Pi_h(w) - w\|_{L^1(K)} \le Ch|w|_{W^{1,1}(K)}\,. \tag{5.88}$$

Hence,

$$\|\Pi_h(v_h^2) - v_h^2\|_{L^1(K)} \le Ch|v_h^2|_{W^{1,1}(K)} \le 2Ch\|v_h\|_{L^\infty}|v_h|_{W^{1,1}(K)}\,.$$

As $0 \le v_h \le 1$ and v_h is bounded in $H^1(\omega)$, we have $\|\Pi_h(v_h^2) - v_h^2\|_{L^1(\omega)} \le Ch$. Since $v_h^2 \to v^2$ in $L^1(\omega)$ we get that $\Pi_h(v_h^2) \to v^2$ in $L^1(\omega)$, and actually in $L^q(\omega)$ for every $1 \le q < \infty$.

Knowing that $v_h \rightharpoonup v$ in $H^1(\omega)$, $\Pi_h(v_h^2) \to v^2$ in $L^1(\omega)$ and $u_h \to u$ in $\mathcal{U}$ it is easy to check that $\mathcal{F}(u,v) \le \liminf_{h\to 0} \mathcal{F}_h(u_h, v_h)$.

Let us fix $\varphi \in C^\infty(\bar\omega)$ with $\varphi \le 0$ and $\|\varphi\|_{L^2} \le 1$. Denote $\varphi_h = \Pi_h\varphi$. First, let us check that $\|\varphi_h\|_{\mathcal{V}_h} \to \|\varphi\|_{L^2}$. By classical interpolation estimates, $\varphi_h \to \varphi$ in $H^1(\omega)$ and thus $\|\varphi_h\|_{L^2} \to \|\varphi\|_{L^2}$. Remember that $\|\varphi_h\|_{\mathcal{V}_h} = \|\Pi_h(\varphi_h^2)\|_{L^1}^{1/2}$. Moreover, using the interpolation estimate (5.88), we get

$$\|\Pi_h(\varphi_h^2) - \varphi_h^2\|_{L^1} \leq Ch\|\varphi_h\|_{L^\infty}|\varphi_h|_{W^{1,1}} \leq C'h,$$

for some $C' > 0$ independent of h. Hence,

$$\left|\|\varphi_h\|_{L^2}^2 - \|\varphi_h\|_{\mathcal{V}_h}^2\right| = \left|\|\varphi_h^2\|_{L^1} - \|\Pi_h(\varphi_h^2)\|_{L^1}\right| \leq C'h\,,$$

which implies that $\|\varphi_h\|_{\mathcal{V}_h} \to \|\varphi\|_{L^2}$. We now define the sequence

$$\hat{\varphi}_h := \begin{cases} \frac{\varphi_h}{\|\varphi_h\|_{\mathcal{V}_h}} & \text{if } \|\varphi\|_{L^2} = 1\,, \\ \varphi_h & \text{if} \|\varphi\|_{L^2} < 1\,. \end{cases}$$

Clearly, $\hat{\varphi}_h \in \mathcal{V}_h$ and $\hat{\varphi}_h \leq 0$ in ω. Since $\varphi_h \to \varphi$ in $H^1(\omega)$ and $\|\varphi_h\|_{\mathcal{V}_h} \to \|\varphi\|_{L^2}$, we also have that $\hat{\varphi}_h \to \varphi$ in $H^1(\omega)$ and, for h small enough, that $\|\hat{\varphi}_h\|_{\mathcal{V}_h} \leq 1$. Hence $\hat{\varphi}_h$ is an admissible test function in (5.52) and

$$\partial_v \mathcal{F}_h(u_h, v_h)[\hat{\varphi}_h] = \int_\omega \Pi_h(v_h\hat{\varphi}_h)\nabla u_h^\top A_1 \nabla u_h \,\mathrm{d}x + \int_\omega \nabla v_h^\top A_2 \nabla \hat{\varphi}_h \,\mathrm{d}x - \int_\omega \Pi_h((1-v_h)\hat{\varphi}_h)\,\mathrm{d}x\,.$$

Using again the interpolation estimate (5.88) we get

$$\|\Pi_h(v_h\hat{\varphi}_h) - v_h\hat{\varphi}_h\|_{L^1} \leq Ch\|v_h\hat{\varphi}_h\|_{L^\infty}\,|v_h\hat{\varphi}_h|_{W^{1,1}} \leq C'h.$$

Since $v_h\hat{\varphi}_h \to v\varphi$ in $L^1(\omega)$ we get that $\Pi_h(v_h\hat{\varphi}_h) \to v\varphi$ in $L^1(\omega)$. Remembering that $v_h \rightharpoonup v$ in $H^1(\omega)$ and that $u_h \to u$ in $\mathcal{U}$ it is easy to check that

$$\liminf_{h\to 0} |\partial_v^- \mathcal{F}_h|_{\mathcal{V}_h}(u_h, v_h) \geq \liminf_{h\to 0} -\partial_v \mathcal{F}_h(u_h, v_h)[\hat{\varphi}_h] = -\partial_v \mathcal{F}(u, v)[\varphi]\,.$$

Passing to the supremum over φ we conclude the proof. □

We are now ready to prove Theorem 5.4.18.

Proof of Theorem 5.4.18. First, let us see, briefly, that $u_{0,h} \to u_0$ in $\mathcal{U}$. By minimality there holds

$$\mathcal{E}_h(u_{0,h}, v_{0,h}) \leq \mathcal{E}_h(g_{0,h}, v_{0,h}) \leq C(1+\eta)\|g_{0,h}\|_{H^1}\,.$$

By (5.10) $u_{0,h}$ is bounded in $\mathcal{U}$. Up to subsequences, not relabelled, $u_{0,h} \rightharpoonup w$ in $\mathcal{U}$. Since $\Pi_h(v_{0,h}^2) \to v_0^2$ in $L^1(\omega)$, using the Euler-Lagrange equations and the arguments of Lemma 5.2.4, it is not difficult to check that $w = u_0$ and that $u_{0,h} \to u_0$ in $\mathcal{U}$.

Let $(u_h, v_h)\colon [0,T] \to \mathcal{U}_h \times \mathcal{V}_h$ be as in the statement of the theorem. In view of Definition 5.4.9, we have that the sequence u_h is bounded in $L^\infty([0,T];\mathcal{U})$, while the sequence v_h is bounded in $L^\infty([0,T];H^1(\omega))$ and in $H^1([0,T];L^2(\omega))$. Therefore, there exists $v \in H^1([0,T];L^2(\omega))$ such that $v_h \rightharpoonup v$ weakly in $H^1([0,T];L^2(\omega))$. With the same argument used in the proof of Theorem 5.3.5 in Section 5.3, we can also show that $v_h(t) \rightharpoonup v(t)$ weakly in $H^1(\omega)$ for every $t \in [0,T]$.

Applying [2, Lemma 5.2], we have that there exists $u \in L^\infty([0,T];\mathcal{U})$ such that $u_h(t) \to u(t)$ in $\mathcal{U}$ for every $t \in [0,T]$ and such that the pair $(u(t), v(t))$ satisfies the displacement equilibrium property (c) of Definition 5.1.5. The time regularity of u follows by Lemma 5.2.4 and by the regularity of v.

Passing to the lim inf in the energy inequality (d) of Definition 5.4.9, by the convergences shown above, by the hypotheses of the theorem, and by Lemma 5.4.19, we immediately get

$$\mathcal{F}\big(u(t),v(t)\big) \le \mathcal{F}(u_0,v_0) - \frac{1}{2}\int_0^t \big\|\dot v(s)\big\|_2^2 + |\partial_v^- \mathcal{F}|^2\big(u(s),v(s)\big)\,\mathrm{d}s + \int_0^t \mathcal{P}\big(u(s),v(s),\dot g(s)\big)\,\mathrm{d}s\,.$$

The opposite inequality follows by Proposition 5.1.9. □

5.5 One vs. Multi Step Scheme

In this section we present some numerical experiments to show the applicability of the discrete schemes studied in Section 6. Our aim is to compare the efficiency of the one-step and multi-step schemes, validating the choices and the analysis made in the previous theoretical sections. However, for simplicity we will only consider the anti-plain strain setting here. Thus, in (5.1) we have $b = 0$ and $A_1 = A_2 = \mathrm{Id}$.

In the first simulations, we compare the evolutions obtained by one-step and multi-step algorithm in a geometrically simple setting. For both schemes, we will apply the alternate minimization algorithm of Section 6 with $J = 1$ and $J \gg 1$, respectively (J being the upper bound on the number of iterations). We will see that, from a computational point of view, the multi-step scheme with an appropriate stopping criterion is the right choice. Indeed, it provides good solutions in a large range of time steps, while the one-step scheme seems to fail in some cases, for instance when the propagation is very fast (in our experiments when the crack reaches the boundary of the domain). Then, we briefly show some simulations, based only on the multi-step scheme, in which the crack path kinks and curves. All the simulations are computed using the partial differential solver `FreeFEM` [78].

Before showing examples we fix some details, describing the general numerical framework and how the alternate minimization schemes are precisely implemented. The finite dimensional energy functional is given by

$$\mathcal{F}_{\varepsilon,h}(u,v) := \frac{1}{2}\int_\omega (\Pi_h(v^2)+\eta_\varepsilon)|\nabla u|^2\,\mathrm{d}x + \frac{\kappa}{4\varepsilon}\int_\omega \Pi_h\big((1-v)^2\big)\,\mathrm{d}x + \kappa\varepsilon\int_\omega |\nabla v|^2\,\mathrm{d}x\,,$$

where $0 < \eta_\varepsilon \ll \varepsilon \ll 1$ are approximating parameters (related to the Γ-convergence of the Ambrosio-Tortorelli functional [12]) and $\kappa > 0$ is the toughness. Note that, for notational convenience, in the previous sections we have set, without loss of generality, $\kappa = 1$ and $\varepsilon = \frac{1}{2}$. For the following numerical experiments we keep $\kappa = 1$ fixed and use $\varepsilon = 5 \cdot 10^{-3}$ and $\eta_\varepsilon = 10^{-5}$.

Given a final time $T > 0$, the interval $[0, T]$ is discretized by a constant time step $\tau = (T/k) > 0$ (for some $k \gg 1$) so that we set $t_0 := 0$ and $t_i := i\tau$ for $1 \le i \le k$. In both the algorithms we are going to define u_i and v_i as in (5.60)–(5.62). Actually, the phase field minimization in (5.61) is then performed with respect to the functional

$$\mathcal{F}_{\varepsilon,h}(u, v) + \frac{\alpha}{\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h}, \quad \text{for } \alpha > 0.$$

Note that, without loss of generality, in the previous sections we used $\alpha = \frac{1}{2}$. For our purposes we set $\alpha = 10^{-3}$, indeed here the L^2-gradient flow is intended as vanishing viscosity approximation for a quasi-static BV-evolution (see e.g. [98]).

The alternate minimizing iterations, with respect to the index j, are interrupted when $\|v_{i,j} - v_{i,j-1}\|_{L^\infty}$ is smaller than a certain threshold, which we call $\texttt{TOL}_v$ and fix to the value $2 \cdot 10^{-3}$. In practice, the assumption of a uniform bound for the number of iterations, as required in Section 5.4, is not imposed; indeed, we will see that the stopping criterion is always reached and that the number of iterations, at each time step, is decreasing as τ becomes smaller. Therefore, we expect, a posteriori, that the number of iterations is again uniformly bounded with respect to τ.

On most parts of the domain the phase field function will be nearly constant. Only close to the crack it is expected to be very steep. To get an appropriate interpolation error, the mesh has to be very fine in the neighborhood of the crack, while it can be coarse elsewhere. Thus, we use an adaptive triangulation refining the mesh where it is necessary. Such approaches have been investigated accurately in [16, 38]. For our purposes, we regularly adapt the mesh in the iteration procedure using the standard routine `adaptmesh` provided from `FreeFEM`, which uses a standard anisotropic second order interpolation error estimate. We fix the error tolerance $\texttt{TOL}_{\text{ref}} = 10^{-3}$.

Algorithm 5.1 Implementation of the one-step scheme with mesh adaptation.

initialize v_0
for $i = 1$ to k **do**
  repeat
    $u_i \leftarrow \arg\min\{\mathcal{E}_h(u, v_{i-1}) : u \in \mathcal{U}_h, u = g(t_i) \text{ on } \partial\omega\}$
    $v_i \leftarrow \arg\min\left\{\mathcal{F}_h(u_i, v) + \frac{\alpha}{\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h\right\}$
    $v_i \leftarrow \min\{v_i, v_{i-1}\}$
    mesh adaption with error tolerance $\texttt{TOL}_{\text{ref}}$
  until "relative change of nodes" $<$ $\texttt{TOL}_{\text{adapt}}$
end for

Algorithm 5.2 Implementation of the multi-step scheme with mesh adaptation.

initialize v_0
$\tilde{v}_0 \leftarrow v_0$
for $i = 1$ to k **do**
  repeat
    $j \leftarrow 0$
    repeat
      $j \leftarrow j + 1$
      $\tilde{u}_j \leftarrow \arg\min\{\mathcal{E}_h(u, \tilde{v}_{j-1}) : u \in \mathcal{U}_h, u = g(t_i) \text{ on } \partial\omega\}$
      $\tilde{v}_j \leftarrow \arg\min\left\{\mathcal{F}_h(\tilde{u}_j, v) + \frac{\alpha}{\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h\right\}$
      $\tilde{v}_j \leftarrow \min\{\tilde{v}_j, v_{i-1}\}$
    until $\|\tilde{v}_j - \tilde{v}_{j-1}\|_\infty < \mathtt{TOL}_v$ **or** $j = 10$
    mesh adaption with error tolerance $\mathtt{TOL}_{\text{ref}}$
    $\tilde{v}_0 \leftarrow \tilde{v}_j$
  until "relative change of nodes" $< \mathtt{TOL}_{\text{adapt}}$ **and** $\|\tilde{v}_j - \tilde{v}_{j-1}\|_\infty < \mathtt{TOL}_v$
  $v_i \leftarrow \tilde{v}_j$
  $u_i \leftarrow \tilde{u}_j$
end for

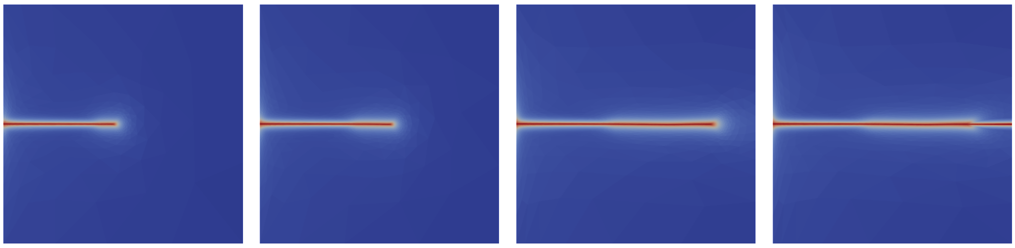
Table 5.1: Numerical Parameters.

λ	μ	κ	ε	η_ε	α	$\mathtt{TOL}_{\text{ref}}$	$\mathtt{TOL}_{\text{adapt}}$	$\mathtt{TOL}_v$
0	1	1	$5 \cdot 10^{-3}$	10^{-5}	10^{-3}	10^{-2}	10^{-2}	$2 \cdot 10^{-3}$

The complete algorithms in the way how we implement them for the presented experiments are given in detail by Algorithm 5.1 and Algorithm 5.2. All the appearing parameters and variables, which are fixed throughout the section, are summarized in Table 5.1.

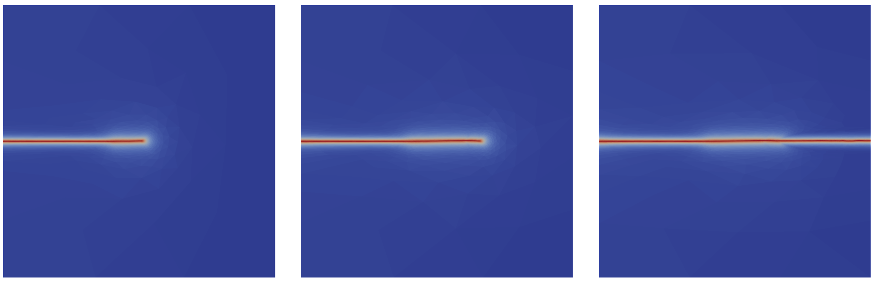
Let us fix the domain, the boundary condition and the initial configuration. The domain ω is given by $(0,1) \times (0,1)$ and we impose a boundary condition on $\{0\} \times (0,1)$. Furthermore, we consider a pre-existing crack given by the line segment with extrema $(0,0.5)$ and $(0.4,0.5)$. In the phase field setting, the pre-crack is represented by the initial condition v_0. To this end we use the optimal profile functions rescaled by $\varepsilon > 0$. Precisely, we define

$$v_0(x,y) := \begin{cases} 1 - \exp\left(\frac{-|y-0.5|}{\varepsilon}\right) & \text{if } x < 0.4\,, \\ 1 - \exp\left(\frac{-\sqrt{(y-0.5)^2+(x-0.4)^2}}{\varepsilon}\right) & \text{if } x \geq 0.4\,. \end{cases} \tag{5.89}$$



(a) $t = 1.2$ (b) $t = 1.35$ (c) $t = 1.574$ (d) $t = 1.575$

Figure 5.1: Phase field at different times using the one step scheme with time step size $\tau = 10^{-3}$, the boundary condition g from (5.90) and the initial phase field v_0 from (5.89).



(a) $t = 1.2$ (b) $t = 1.35$ (c) $t = 1.36$

Figure 5.2: Phase field at different times using the multi step scheme with time step size $\tau = 10^{-2}$, the boundary condition g from (5.90) and the initial phase field v_0 from (5.89).

Note, that this choice has been well elaborated. In order to show the Γ-lim sup-inequality of the Γ-convergence statement in Theorem 4.1.2, precisely this function was used as a recovery sequence (assuming $\eta_\varepsilon = 0$) in the proof of Proposition 4.1.5.

For the first example, we consider a symmetric setting, pulling the upper hole B^+ up and the lower hole B^- down monotonically in time. Concretely, we consider the Dirichlet condition

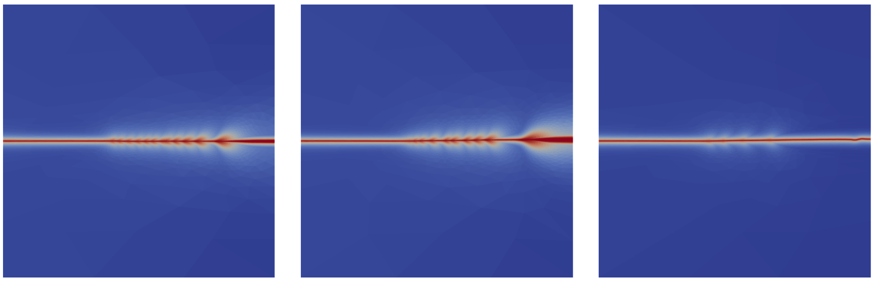
$$g(t) = \begin{cases} (0,t) & \text{on } \partial B^+ , \\ (0,-t) & \text{on } \partial B^- . \end{cases} \tag{5.90}$$

Figure 5.1 and Figure 5.2 show the phase field for the one-step scheme with $\tau = 10^{-3}$ and for the multi-step scheme with $\tau = 10^{-2}$, respectively.

As already mentioned in the introduction of this chapter, we expect the multi-step scheme to converge faster with respect to the time step τ, since in this algorithm we approximate a critical point of the energy functional for each time node. In order to investigate this phenomenon, we perform the simulation for several time step sizes and compare in Table 5.2 the time when the crack is completed, i.e., when the domain is split in two subdomains and the elastic energy vanishes. Furthermore, in order to compare efficiency, in Table 5.2 we also show the number of iterations. Note that, due to the mesh adaptation, the number of iterations in the one-step scheme exceeds the number of time nodes.

Table 5.2: Calculation time and the time t when the crack completes for different time step sizes τ.

	time step size τ	10^{-1}	$5 \cdot 10^{-2}$	$2 \cdot 10^{-2}$	10^{-2}	$5 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	10^{-3}
time of crack completion	single step	2.2	2.05	2.04	1.78	1.79	1.622	1.575
	multi step	1.4	1.35	1.36	1.36	1.365	1.37	1.387
number of iterations	single step	120	157	203	281	423	881	1650
	multi step	1148	1961	2951	3491	3835	4853	5912



(a) One step scheme with $\tau = 0.05$.

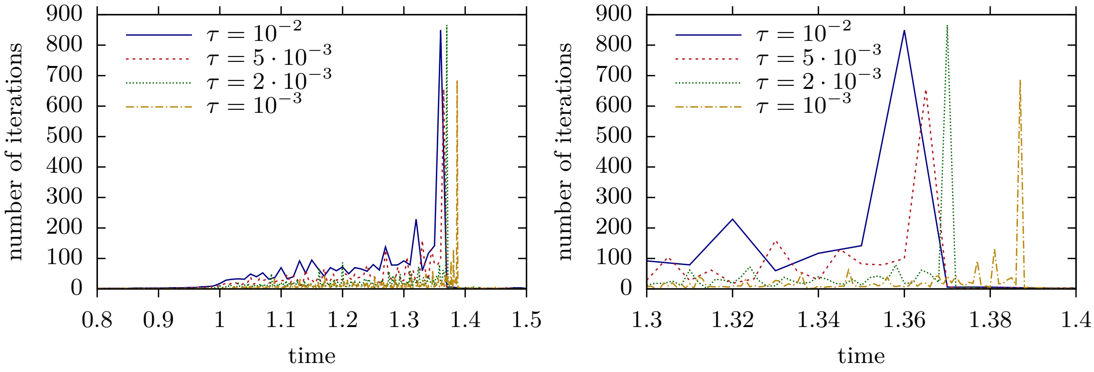
(b) One step scheme with $\tau = 0.1$.

(c) Multi step scheme with $\tau = 0.1$.

Figure 5.3: Comparison of final phase fields with big time step sizes.

We notice that, in the one-step scheme, for $\tau \geq 0.05$ we get a qualitatively poor solution. Indeed, as shown in Figure 5.3, the crack spreads too much in the bulk. From Table 5.2 it is also clear that the time of crack completion decreases as the time step size decreases. On the contrary, with the multi-step scheme the crack always completes at around $t = 1.36$ and solutions are qualitatively very good even for $\tau = 0.1$.

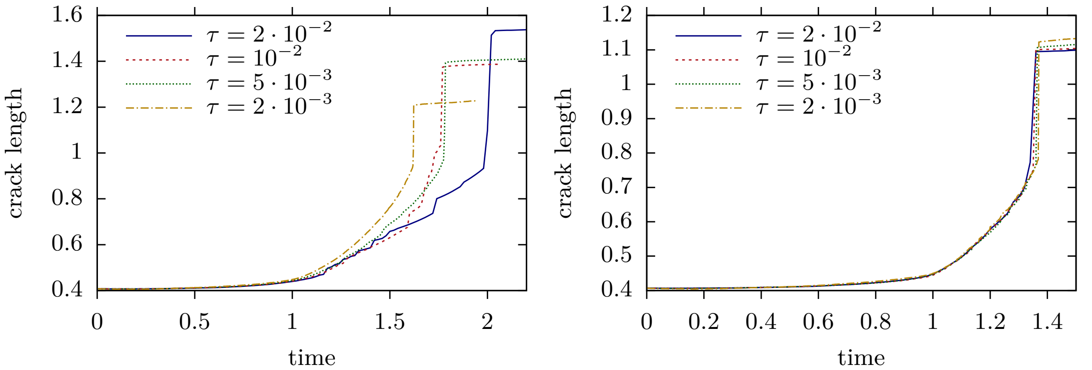
In Figure 5.4 we plot, as a function of t_i, the number of iterations needed by the multi-step scheme to fulfill the stopping criterion. It is clear that the smaller the time step size the less iterations are needed. For τ small enough the multi-step scheme fulfills the stopping criterion more or less after one iteration until the time node t_i where the last part of the crack appears almost instantaneously is reached. At this node the number of iteration blows up. In Figure 5.5 we show the crack length as a function of time variable. The length of the fracture is estimated by the dissipative energy $\int_\omega \frac{1}{4\varepsilon}(1-v)^2 + \varepsilon|\nabla v|^2 \,\mathrm{d}x$. The physical maximum crack length of 1 is exceeded due to interpolation errors and diffusions of the phase field. We notice that, also in this plot, the last part of the crack is well visible as a jump in the evolution.



(a) $t \in [0.8, 1.5]$.

(b) Zoomed in for $t \in [1.3, 1.4]$.

Figure 5.4: Number of iterations, as a function of time, using the multi-step scheme for different time step sizes, for the boundary condition g from (5.90) and for the initial phase field v_0 from (5.89).



(a) One Step Scheme.

(b) Multi Step Scheme.

Figure 5.5: Crack length at each time step for different time step sizes, for the boundary condition g from (5.90) and for the initial phase field v_0 from (5.89).

6 Mesh Adaption and Numerical Computation

In fracture simulation adaptive mesh procedures increase the efficiency of the computation enormously, which is due to the fact that the mesh only needs to be fine enough nearby the crack, where the phase field and displacement have a rather high gradient. As the crack path is not known in advance it is a natural idea to use an adaptive procedure during the alternating minimization scheme. In this chapter we present an anisotropic mesh adaption based on a residual estimate, as it has been presented in [16, 38] for the planar case, and we show some numerical example of brittle fracture of some elastic shells. The anisotropy which we take into account exploits the fact, that the mesh can be well aligned along the crack path, since it needs mainly to refine in the orthogonal direction of the fracture.

The theory of this chapter is discussed – as in Chapter 5 – for phase-field models of the form

$$\mathcal{F}(u,v) := \mathcal{E}(u,v) + \mathcal{D}(v) \tag{6.1}$$

where we set for all $u \in H^1(\omega)$, $v \in H^1(\omega;[0,1])$

$$\begin{aligned}\mathcal{E}(u,v) &:= \frac{1}{2}\int_\omega b|u|^2 \,\mathrm{d}x + \frac{1}{2}\int_\omega (v^2+\eta)\nabla u^\top A_1 \nabla u \,\mathrm{d}x\\ \mathcal{D}(u,v) &:= \kappa \int_\omega \frac{1}{4\varepsilon}(1-v)^2 K + \varepsilon\, \nabla v^\top A_2 \nabla v \,\mathrm{d}x\,.\end{aligned}$$

Again, A_1, A_2 are symmetric, positive definite matrix functions and K, b are real non-negative functions. The approximation parameter $\varepsilon > 0$ and $\eta > 0$ shall be fixed. As shown in the introduction of Chapter 5 we can later on simply apply our phase field model for thin shells, which we derived in Section 4.2, to this setting by the right choice of A_1, A_2, K and b. Naturally, when doing numerical analysis, the functional has to be discretized, which we do by a finite element method, which has been already introduced in Section 5.4.1. We recall the main core in Section 6.1.

A crucial part of this chapter is the anisotropic mesh adaption that we include in our numerical scheme. Such mesh adaption procedures has been established in [38, 39]. They are based on the fact that on the finite element space a critical point is computed, for instance by the alternating minimization (5.2)–(5.3) (see [16, 38]). One then estimates, roughly speaking, how far this solution is from fulfilling the condition of being a critical point in the infinite dimensional function space. In this way we obtain some residual estimates which serve as the basis for our mesh creation. We need to admit that repeating the multi-step scheme introduced in (5.60)–(5.61) in Section 5.4.2 infinitely many times, does not provably result in a critical point. However, we note that the constraint alternating minimization (5.2)–(5.3) does so. Here, it is also possible to replace $v^k_{i,j-1}$ by v^k_{i-1} in the inequality constraint as it has been – at least partially – done in [40]. In our experiment we kind of mix the two approaches by using the L^2-penalization when minimizing with respect to u in (5.61) but using the inequality constrained $v \leq v^k_{i-1}$. Being more precise, for some boundary data $g \in AC([0,T], W^{1,p}(\omega))$ with $p > 2$ and for given $u_0 \in H^1(\omega)$, $v_0 \in H^1(\omega; [0,1])$ with $u_0 = g(0)$, we set for all $i, j \in \mathbb{N}$ inductively $u_{i,0} = u_{i-1}$, $v_{i,0} = v_{i-1}$ and

$$u_{i,j} := \arg\min\{\mathcal{E}(u, v_{i,j-1}) : u \in H^1(\omega), u = g(t^k_i) \text{ on } \partial\omega\}\,, \tag{6.2}$$

$$v_{i,j} := \arg\min\left\{\mathcal{F}(u_{i,j}, v) + \frac{\alpha}{2\tau}\|v - v_{i-1}\|^2_{L^2(\omega)} : v \in H^1(\omega), 0 \leq v \leq v_i\right\}. \tag{6.3}$$

One can prove, as in Proposition 6.1.4, that for each $i \in \mathbb{N}$ we get a critical point as $j \to \infty$ (see [39, Proposition 2]), so that we can further set

$$u_i = \lim_{j\to\infty} u_{i,j} \quad \text{and} \quad v_i = \lim_{j\to\infty} v_{i,j} \tag{6.4}$$

We believe that in this setting Chapter 5 can be repeated almost literally in order to obtain also in this case a unilateral L^2-gradient flow in the sense of Definition 5.1.5 and Definition 5.4.9.

In Section 6.2.3 we establish paritcularly for this scheme the mentioned residual estimates, where the anisotropic information is gained from some anisotropic interpolation estimates (see [14, 65]). Provided that there is an initial mesh available, we construct a new mesh following the general idea of finding the triangulation with the least number of elements, which still estimates the residual to a certain precision. To this end we follow the strategy of a metric based mesh construction, which has been successfully used for many different problems (see e.g. [66, 91, 92, 93]). We describe the procedure more detailed in Section 6.3.

The content of this chapter was developed in cooperation with Stefano Micheletti and Simona Perotto. We plan to publish it in combination with Chapter 3 in the paper [4] after the submission of this thesis.

6.1 The Discrete Setting

Let us briefly recall the time and space discretization as already described in Chapter 5. In this way we also declare some notations and the precise algorithm which we apply in the numerical examples shown in Section 6.4.

The space discretization is done by an finite element method. As in Section 5.4.1 we consider a polyhedral set $\omega \in \mathbb{R}^2$ and a triangulation denoted by $\mathcal{T}_h$. For any triangle $T \in \mathcal{T}_h$, Δ_T denotes the union of all triangles sharing at least one vertex with T. The diameter of some triangle $T \in \mathcal{T}_h$ will be written as h_T. Furthermore, the set of all edges of $\mathcal{T}_h$ is denoted by E_h, and h_e is the length of the edge $e \in E_h$.

We define the discretized versions of the function space of $H^1(\omega)$ and $H^1(\omega;[0,1])$ containing all smooth, piecewise affine functions on ω. Precisely, we set

$$\mathcal{U}_h := \left\{u \in H^1(\omega) \colon \nabla u|_T \text{ is constant on } T \text{ for all } T \in \mathcal{T}_h\right\},$$
$$\mathcal{V}_h := \left\{v \in H^1(\omega) \colon \nabla v|_T \text{ is constant on } T \text{ for all } T \in \mathcal{T}_h, 0 \leq v \leq 1\right\}.$$

On these spaces we define the discretized version of $\mathcal{F}$ from (6.1) by

$$\mathcal{F}_h(u,v) := \mathcal{E}_h(u,v) + \mathcal{D}_h(v) \quad \text{for all } u \in \mathcal{U}_h, v \in \mathcal{V}_h$$

with

$$\mathcal{E}_h(u,v) = \frac{1}{2}\int_\omega b|u|^2 \,\mathrm{d}x + \frac{1}{2}\int_\omega (\Pi_h(v^2)+\eta)\nabla u^\top A_1 \nabla u \,\mathrm{d}x$$
$$\mathcal{D}_h(v) = \int_\omega \frac{1}{4\varepsilon}\Pi_h((1-v)^2)K + \varepsilon\, \nabla v^\top A_2 \nabla v \,\mathrm{d}x\,.$$

Again, Π_h denotes the standard nodal interpolation operator. Its presence ensures, that when minimizing the energy with respect to v the minimizer is automatically in the interval $[0,1]$ (see Remark 5.4.4). As in Section 5.4.1 we use as special norm on $\mathcal{V}_h$ defined by

$$\|v\|_{\mathcal{V}_h} = \left(\int_\omega \Pi_h(v^2)\,\mathrm{d}x\right)^{\frac{1}{2}} \quad \text{for all } v \in \mathcal{V}_h\,.$$

We now describe the numerical scheme that we use for our numerical computations. For a given time increment $\tau > 0$ we define the time steps $t_i = i\tau$ for $i \in \{0,\dots,N\}$ for some $N \in \mathbb{N}$. Let $g \in AC([0,N\tau];W^{1,p}(\omega))$ for some $p > 2$ describing the time dependent boundary condition for our displacement function. Our alternating minimization scheme now works as follows: Suppose that $u_0 \in \mathcal{U}_h$ and $v_0 \in \mathcal{V}_h$ are given. Then for all $i,j \in \mathbb{N}$ we inductively set $u_{i,0} = u_{i-1}$, $v_{i,0} = v_{i-1}$ and

$$u_{i,j} := \arg\min\{\mathcal{E}_h(u, v_{i,j-1}) : u \in \mathcal{U}_h, u = g(t_i^k) \text{ on } \partial\omega\}\,, \tag{6.5}$$
$$v_{i,j} := \arg\min\left\{\mathcal{F}_h(u_{i,j}, v) + \frac{\alpha}{2\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h, v \leq v_i\right\}. \tag{6.6}$$

As shown in Proposition 6.1.4 below, there exists a subsequence j_k such that (u_{i,j_k}, v_{i,j_k}) converges to some (u_i, v_i) as $k \to \infty$. Thus, we can set

$$u_i = \lim_{k\to\infty} u_{i,j_k} \quad \text{and} \quad v_i = \lim_{k\to\infty} v_{i,j_k}\,. \tag{6.7}$$

Once more we clarify that with the pointwise minimization (5.62) we would not be able to prove the convergence, so that the last step (6.7) would make sense. Nevertheless, we believe that the convergence to a unilateral L^2-gradient flow of this scheme can be shown like in Chapter 5. The additional parameter α is chosen rather small and does not change the analysis of the time-evolution theory. Like in Section 5.5, we rather intend a vanishing viscosity approach in order to obtain a quasi-static evolution along critical points.

Note that $\mathcal{F}_h(u,v)$ is Fréchet differentiable (see e.g. [38, Proposition 1.1]) with

$$\partial_u \mathcal{F}_h(u,v)[\psi] = \partial_u \mathcal{E}_h(u,v;\psi) = \int_\omega bu\psi \,\mathrm{d}x + \int_\omega (\Pi_h(v^2)+\eta)\nabla u^\top A_1 \nabla\psi \,\mathrm{d}x$$

for all $u,\psi \in \mathcal{U}_h$, $v \in \mathcal{V}_h$ and

$$\partial_v \mathcal{F}_h(u,v)[\psi] = \int_\omega \Pi_h(v\psi)\nabla u^\top A_1 \nabla u \,\mathrm{d}x - \int_\omega \frac{1}{2\varepsilon}\Pi_h\big((1-v)\psi\big)K + 2\varepsilon\,\nabla v^\top A_2 \nabla\psi \,\mathrm{d}x\,.$$

for all $u \in \mathcal{U}_h$, $v,\psi \in \mathcal{V}_h$.

A critical point with respect to the minimization (6.5) and (6.6) can, hence, be defined in the following way, where we also need to take care of the L^2-penalization term in (6.6).

Definition 6.1.1. Let $u \in \mathcal{U}_h$, $v,\tilde{v} \in \mathcal{V}_h$. We say that (u,v) is a critical point if the following two conditions hold

$$\partial_u \mathcal{E}_h(u,v)[\psi_1] = 0\,, \tag{6.8}$$

$$\partial_v \mathcal{F}_h(u,v)[v-\psi_2] + \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v-\tilde{v})(v-\psi_2)\big)\,\mathrm{d}x \le 0\,, \tag{6.9}$$

for all $\psi_1 \in \mathcal{U}_h$ with $\psi_1 = 0$ on $\partial\omega$ and for all $\psi_2 \in \mathcal{V}_h$ with $\psi_2 \le \tilde{v}$.

Remark 6.1.2. Note that, since $u \mapsto \mathcal{F}_h(u,v)$ is convex the minimization of the displacement variable in (6.5) is equivalent to (6.8). The inequality condition (6.9) is due to the inequality constraint in (6.6). In fact, since $v \mapsto \mathcal{F}_h(u,v)$ is convex also (6.9) is equivalent to the minimization of the phase field variable in (6.6) with v_{i-1} replaced by $\tilde{v}$ (cf. [85, Chapter 3]).

Remark 6.1.3. By the right choice of ψ_1 and ψ_2 one can easily deduce that (6.8) together with (6.9) is equivalent to the single inequality

$$\partial_u \mathcal{E}_h(u,v)[\psi_1] + \partial_v \mathcal{F}_h(u,v)[v-\psi_2] + \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v-\tilde{v})(v-\psi_2)\big)\,\mathrm{d}x \le 0\,,$$

for all $\psi_1 \in \mathcal{U}_h$ with $\psi_1 = 0$ on $\partial\omega$ and for all $\psi_2 \in \mathcal{V}_h$ with $\psi_2 \le \tilde{v}$.

Following the idea of [39, Proposition 2] we show the convergence of the solutions of our minimization scheme to a critical point in the sense of the previous definition. The result can easily be extended to the space-continuous scheme (6.2)–(6.4).

Proposition 6.1.4. *For given $u_0 \in \mathcal{U}_h$ and $v_0 \in \mathcal{V}_h$ let $(u_{i,j}, v_{i,j})$ be defined as in* (6.5)–(6.6)*. Then $(u_{i,j}, v_{i,j})$ converges, up to a subsequence, as $j \to \infty$ to a critical point (u_i, v_i).*

Proof. Let $(u_j, v_j) := (u_{i,j}, v_{i,j})$ be given as in (6.5)–(6.6). Due to the minimization scheme we have for all $j \in \mathbb{N}$

$$\begin{aligned}\mathcal{F}_h(u_j, v_j) + \frac{\alpha}{2\tau}\|v_j - v_{i-1}\|^2_{\mathcal{V}_h} &\le \mathcal{F}_h(u_{j-1}, v_{j-1}) + \frac{\alpha}{2\tau}\|v_{j-1} - v_{i-1}\|^2_{\mathcal{V}_h} \\ &\le \mathcal{F}_h(u_0, v_0) + \frac{\alpha}{2\tau}\|v_0 - v_{i-1}\|^2_{\mathcal{V}_h}\,.\end{aligned}$$

Since A_1 and A_2 are uniformly positive definite we get that (u_j, v_j) is bounded in $\mathcal{U}_h \times \mathcal{V}_h$. Hence, we can extract a subsequence j_k such that for some $u \in \mathcal{U}_h$, $v, \tilde{v} \in \mathcal{V}_h$ we have

$$\nabla u_{j_k} \to \nabla u\,, \quad v_{j_k} \to v\,, \quad v_{j_k-1} \to \tilde{v} \quad \text{ as } k \to \infty\,.$$

This also implies $u_{j_k-1} \to u$ as $k \to \infty$.

We will now proof that (u, v) is a critical point. In view of Remark 6.1.2 there holds for all $k \in \mathbb{N}$ and for all $\psi_1 \in \mathcal{U}_h$, $\psi_2 \in \mathcal{V}_h$ with $\psi_1 = 0$ on $\partial\omega$ and $\psi_2 \le v_{i-1}$

$$\begin{aligned}&0 = \partial_u \mathcal{E}_h(u_{j_k}, v_{j_k-1})[\psi_1]\,, \\ &0 \le \partial_v \mathcal{F}_h(u_{j_k}, v_{j_k})[\psi_2 - v_{j_k}] + \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v_{j_k} - v_{i-1})(\psi_2 - v_{j_k})\big)\,\mathrm{d}x\,.\end{aligned} \tag{6.10}$$

Taking the limit as $k \to \infty$ it easily follows that

$$\begin{aligned}&0 = \partial_u \mathcal{E}_h(u, \tilde{v})[\psi_1]\,, \\ &0 \le \partial_v \mathcal{F}_h(u, v)[\psi_2 - v] + \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v - v_{i-1})(\psi_2 - v)\big)\,\mathrm{d}x\,.\end{aligned}$$

In order to conclude the proof, there remains to show that $v = \tilde{v}$. Indeed, we have, due to the minimization (6.6)

$$\begin{aligned}\mathcal{F}_h(u, \tilde{v}) + \frac{\alpha}{2\tau}\|\tilde{v} - v_{i-1}\|^2_{X_h} &= \lim_{k\to\infty} \mathcal{F}_h(u_{j_k}, v_{j_k-1}) + \frac{\alpha}{2\tau}\|v_{j_k-1} - v_{i-1}\|^2_{X_h} \\ &\le \lim_{k\to\infty} \mathcal{F}_h(u_{j_{k-1}}, v_{j_{k-1}}) + \frac{\alpha}{2\tau}\|v_{j_{k-1}} - v_{i-1}\|^2_{X_h} \\ &= \mathcal{F}_h(u, v) + \frac{\alpha}{2\tau}\|v - v_{i-1}\|^2_{X_h}\,.\end{aligned}$$

Since (6.6) has a unique solution, which is due to the strict convexity of the functional, there must hold $v = \tilde{v}$. In view to (6.10), (u, v) is, consequently, a critical point. □

6.2 Residual Estimate

In order to preserve the anisotropic information in the residual estimates, we need some anisotropic interpolation results.

We denote by Q_h some quasi-interpolation operator, such as introduced by Clément, Verfürth or Scott-Zhang in [50, 100, 104], for which holds

$$\|u - Q_h u\|_{L^2(T)} \le C h_T \|\nabla u\|_{L^2(\Delta_T)}\,, \tag{6.11}$$

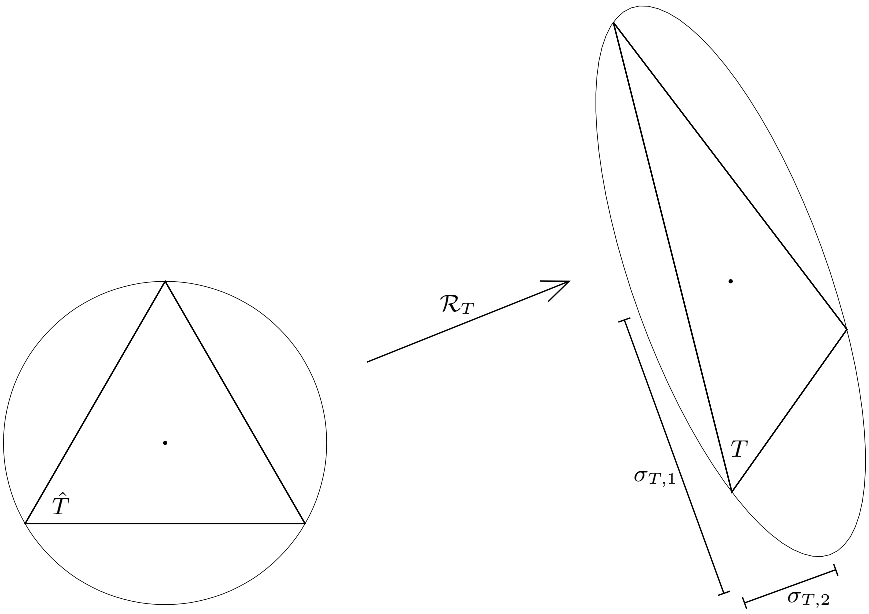


Figure 6.1: Geometrical illustration of the singular value decomposition of the affine map $\mathcal{R}_T$, mapping the uniform reference triangle $\hat{T}$ to T.

$$\|u - Q_h u\|_{H^1(T)} \leq C\|\nabla u\|_{L^2(\Delta_T)}\,, \tag{6.12}$$

where Δ_T denotes the union of all triangles sharing at least one vertex with T, and $h = \operatorname{diam}(T)$. These estimates are standard but do not provide any anisotropic information. We follow the idea of [65] in order to get the anisotropic versions. For this purpose we consider a fixed reference triangle $\hat{T}$. Then, for each $T \in \mathcal{T}_h$ there exists a bijective affine map $\mathcal{R}_T \colon \hat{T} \to T$ with $\mathcal{R}_T(x) = M_T x + \theta_T$ for all $x \in \hat{T}$, where $M_T \in \mathbb{R}^{2\times 2}$ is invertible and $\theta_T \in \mathbb{R}^2$ is the translation vector. In case that $\hat{T}$ is the equilateral triangle inscribed in the unit circle with one vertex at $(0,1)$, and T has the vertices $(x_1, y_1), (x_2, y_2), (x_3, y_3)$, one gets

$$M_T = \frac{1}{3}\begin{pmatrix} \sqrt{3}(x_2 - x_1) & 2x_3 - x_1 - x_2 \\ \sqrt{3}(y_2 - y_1) & 2y_3 - y_1 - y_2 \end{pmatrix} \quad \text{and} \quad \frac{1}{3}\begin{pmatrix} x_1 + x_2 + x_3 \\ y_1 + y_2 + y_3 \end{pmatrix}.$$

We make use of the singular value decomposition of M_T. Thus we consider $U_T, V_T \in \mathbb{R}^{2\times 2}$ orthogonal and $\Sigma_T \in \mathbb{R}^{2\times 2}$ diagonal with entries $\sigma_{T,1} \geq \sigma_{T,2} \geq 0$ such that $M_T = U_T \Sigma_T V_T^\top$. Using a uniform reference triangle, we obtain in this way all the anisotropic information of the triangle T, stored in the singular values $\sigma_{T,1}$ $\sigma_{T,2}$. To be more precise, it is the quotient of the two values which keeps the anisotropic information. If it is one, i.e. $\sigma_{T,1} = \sigma_{T,2}$ the triangle T is uniform, possibly rescaled by $\sigma_{T,1}$ and rotated by the matrices U_T and V_T. If the quotient, however, is very large, T is a rather slim and long triangle. For a geometrical illustration we added Figure 6.1.

For some function $u\colon T \to \mathbb{R}$ we denote in the following by $\hat{u} := u \circ \mathcal{R}_T$ the corresponding function on the reference triangle. Analogously, we set $\hat{e} := \mathcal{R}_T^{-1}(e)$ for all $e \in E_h$. With this at hand we easily infer for all $T \in \mathcal{T}_h$

$$\det(M_T) = \det(\Sigma_T) = \sigma_{T,1}\,\sigma_{T,2} \quad \text{and} \quad |T| = |\hat{T}|\,\sigma_{T,1}\,\sigma_{T,2}\,.$$

In the following lemma we proof the anisotropic interpolation error estimates of the quasi-interpolant Q_h. We only sketch its proof for completeness. It can be found in full detail in [65] and [66].

Lemma 6.2.1. *For every $T \in \mathcal{T}_h$, $e \in E_h$ with $e \in \partial T$ and for every $u \in H^1(\Delta_T)$ there holds*

$$\|u - Q_h u\|_{L^2(T)}^2 \le C h_{\hat{T}}^2\, \|M_T^\top \nabla u\|_{L^2(\Delta_T)}^2 \tag{6.13}$$

$$\|u - Q_h u\|_{L^2(e)}^2 \le C \frac{h_e}{h_{\hat{e}}\,\sigma_{T,1}\,\sigma_{T,2}} \left(\frac{h_{\hat{T}}}{h_{\hat{e}}} + h_{\hat{e}}\right) \|M_T^\top \nabla u\|_{L^2(\Delta_T)}^2\,. \tag{6.14}$$

Proof. Let $T \in \mathcal{T}_h$ and $u \in H^1(\Delta_T)$. We use a change of variable by the affine map defined by the matrix M_T and some translation vector in order to obtain

$$\|u - Q_h u\|_{L^2(T)}^2 = \det(\Sigma_T)\|\hat{u} - \hat{Q}_h \hat{u}\|_{L^2(\hat{T})}^2\,.$$

Using (6.11) on the reference triangle and transforming back the integral using $\nabla\hat{u} = M_T^\top \widehat{\nabla u}$ we get

$$\|u - Q_h\|_{L^2(T)}^2 \le C h_{\hat{T}}^2 \|M_T^\top \nabla u\|_{L^2(\Delta_T)}^2$$

and we conclude (6.13).

In order to show (6.14), we first note that

$$\|u\|_{L^2(e)}^2 = \frac{h_e}{h_{\hat{e}}} \|\hat{u}\|_{L^2(\hat{e})}^2\,,$$

for all $e \in E_h$, with $e \subset \partial T$. By the scaled trace theorem we, therefore, get

$$\|u\|_{L^2(e)}^2 \le C \frac{h_e}{h_{\hat{e}}} \Big(h_{\hat{e}}^{-1} \|\hat{u}\|_{L^2(\hat{T})}^2 + h_{\hat{e}} \|\nabla \hat{u}\|_{L^2(\hat{T})}^2 \Big)$$

We plug in $u - Q_h u$ and apply (6.13) as well as (6.12) in order to deduce (6.14). □

For the nodal interpolation operator, appearing in the discretized version of our energy functional, we also need to compute the anisotropic version of the well-known interpolation estimate (see e.g. [36, 99]), which states that for each $T \in \mathcal{T}_h$ and each function $v \in W^{2,\infty}(T)$ we have

$$\|v - \Pi_h(v)\|_{L^\infty(T)} \le C h_T^2 |v|_{W^{2,\infty}(T)} \quad \text{for all } T \in \mathcal{T}_h\,. \tag{6.15}$$

Here, $|\cdot|_{W^{2,\infty}(T)}$ denotes the standard semi-norm on $W^{2,\infty}(T)$. We briefly show a useful anisotropic estimate based on (6.15).

Lemma 6.2.2. *Let $v_h, \psi_h \in \mathcal{V}_h$ and $T \in \mathcal{T}_h$. Then there holds*

$$\left\|v_h\psi_h - \Pi_h(v_h\psi_h)\right\|_{L^2(T)} \leq C\frac{h_T^2}{\sigma_{T,2}}|\nabla v_h|_{W^{1,\infty}(T)}\left\|M_T^\top \nabla\psi_h\right\|_{L^2(T)} .$$

Proof. By Hölder's inequality and by (6.15) we simply get

$$\begin{aligned}\|v_h\psi_h - P_h(v_h\psi_h)\|_{L^2(T)} &\leq |T|^{\frac{1}{2}} \left\|v_h\psi_h - \Pi_h(v_h\psi_h)\right\|_{L^\infty(T)} \\ &\leq Ch_T^2|T|^{\frac{1}{2}} \left|v_h\psi_h\right|_{W^{2,\infty}(T)} .\end{aligned}$$

Taking into account that any first derivative of v_h and ψ_h is constant, it is easy to see that

$$\begin{aligned}|v_h\psi_h|_{W^{2,\infty}(T)} &= 2\sum_{i,j}\left\|\partial_i v_h\, \partial_j\psi_h\right\|_{L^\infty(T)} \\ &= 2\,|T|^{-\frac{1}{2}}\,|v_h|_{W^{1,\infty}(T)}\sum_j\left\|\partial_j\psi_h\right\|_{L^2(T)} \\ &\leq C\,|T|^{-\frac{1}{2}}\,|v_h|_{W^{1,\infty}(T)}\,\|\nabla\psi_h\|_{L^2(T)} .\end{aligned}$$

The assertion follows now from the fact that $\|\nabla\psi_h\|_{L^2(T)} \leq \frac{1}{\sigma_{T,2}}\|M_T^\top\nabla\psi_h\|_{L^2(T)}$. □

Before we state the residual estimate, we define for every $T \in \mathcal{T}_h$ the following abbreviation, measuring the jump of the gradient along the edges of the triangle T. For each symmetric positive definite matrix $A \in \mathbb{R}^{2\times 2}$ and $u_h \in \mathcal{U}_h$ we set

$$[\![A\nabla u_h]\!] := \begin{cases}\left|\left(\nabla u_h|_T - \nabla u_h|_{T'}\right)^\top A\nu_T\right| & \text{on } e \in E_h \text{ if } \exists T, T' \in \mathcal{T}_h\colon T\cap T' = e\\ 2\left|\nabla u\right|_T^\top A\nu_T\right| & \text{on } e \in E_h \text{ if } \exists T \in \mathcal{T}_h\colon e \subset \partial\omega\cap\partial T .\end{cases}$$

Moreover, for notational convenience we define for each $T \in \mathcal{T}_h$ the function $h_{\partial T}\colon \partial T \to \mathbb{R}$ by $h_{\partial T} = h_e$ on $e \in E_h$, $e \subset \partial T$, almost everywhere. We are now ready to state and prove the announced residual estimates.

Theorem 6.2.3. *Let $u_h \in \mathcal{U}_h$ and $v_h \in \mathcal{V}_h$. If there holds*

$$\partial_u\mathcal{E}_h(u,v)[\psi_h] = 0 \quad \textit{for all } \psi_h \in \mathcal{U}_h \textit{ with } \psi_h = 0 \textit{ on } \partial\omega\,, \tag{6.16}$$

we get the following estimate

$$\left|\partial_u\mathcal{E}(u_h,v_h)[\psi]\right| \leq C\sum_{T\in\mathcal{T}_h}\gamma_T(u_h,v_h)\|M_T^\top\nabla\psi\|_{L^2(\Delta_T)} \quad \textit{for all } \psi\in H_0^1(\omega)\,, \tag{6.17}$$

where

$$\gamma_T(u_h,v_h) := \left\|p(u_h,v_h)\right\|_{L^2(T)} + \frac{1}{\sigma_{T,2}}\left\|(v_h^2 - \Pi_h(v_h^2))A_1\nabla u_h\right\|_{L^2(T)}$$

$$+ \frac{1}{2\sqrt{\sigma_{T,1}\sigma_{T,2}}} \left\| \sqrt{h_{\partial T}} (v_h^2 + \eta_\varepsilon) [\![A_1 \nabla u]\!] \right\|_{L^2(\partial T)}$$

with

$$p(u_h, v_h) := b u_h - 2 v_h \nabla u_h^\top A_1 \nabla v_h - (v_h^2 + \eta_\varepsilon) \nabla u_h \cdot \operatorname{div}(A_1) .$$

If for all $\psi_h \in \mathcal{V}_h$ with $\psi_h \leq \tilde{v}_h$ for some $\tilde{v}_h \in \mathcal{V}_h$ there holds

$$\partial_v \mathcal{F}_h(u_h, v_h)[v_h - \psi_h] + \frac{\alpha}{\tau} \int_\omega \Pi_h\big((v_h - \tilde{v}_h)(v_h - \psi_h)\big) \,\mathrm{d}x \leq 0 , \tag{6.18}$$

we can estimate

$$\begin{aligned} \partial_v \mathcal{F}(u_h, v_h)[v_h - \psi] + \frac{\alpha}{\tau} \int_\omega (v_h - \tilde{v}_h)(v_h - \psi) \,\mathrm{d}x \\ \leq C \sum_{T \in \mathcal{T}_h} \rho_T(u_h, v_h) \big\| M_T^\top \nabla(\psi - v_h) \big\|_{L^2(\Delta_T)} . \end{aligned} \tag{6.19}$$

for all $\psi \in H^1(\Omega)$ with $\psi \leq \tilde{v}_h$, where we define

$$\begin{aligned} \rho_T(u_h, v_h) :=& \| q(u_h, v_h) \|_{L^2(T)} + \frac{\varepsilon}{\sqrt{\sigma_{T,1}\,\sigma_{T,2}}} \left\| \sqrt{h_{\partial T}} [\![A_2 \nabla v_h]\!] \right\|_{L^2(\partial T)} \\ &+ \frac{h_T^2}{\sigma_{T,2}} \left\| \mu \nabla u_h^\top A \nabla u_h + \frac{1}{2\varepsilon} K \right\|_{L^2(T)} |v_h|_{W^{1,\infty}(T)} \\ &+ \frac{\alpha\, h_T^2}{\tau \sigma_{T,2}} \| \nabla (v_h - \tilde{v}_h) \|_{L^2(T)} , \end{aligned}$$

with

$$q(u_h, v_h) := v_h \nabla u_h^\top A_1 \nabla u_h - \frac{1}{2\varepsilon}(1 - v_h) K - 2\varepsilon \nabla v_h \cdot \operatorname{div}(A_2) + \frac{\alpha}{\tau}(v_h - \tilde{v}_h) .$$

Applying the divergence operator div *to a matrix means here to compute the divergence on each row, resulting in a vector.*

Proof. Assume that for some $u_h \in \mathcal{U}_h$, $v_h \in \mathcal{V}_h$ there holds (6.16). Let $\psi_h \in \mathcal{U}_h$ with $\psi_h = 0$ on $\partial\omega$ and $\psi \in H_0^1(\omega)$. Using the linearity of $\psi \to \partial_u G(u_h, v_h)[\psi]$ we simply estimate

$$\big| \partial_u \mathcal{E}(u_h, v_h)[\psi] \big| \leq \big| \partial_u \mathcal{E}(u_h, v_h)[\psi - \psi_h] \big| + \big| \partial_u \mathcal{E}(u_h, v_h)[\psi_h] \big| . \tag{6.20}$$

For the first term on the right hand side we get from the divergence theorem and the fact that $\Delta u_h = 0$

$$\begin{aligned} &\partial_u \mathcal{E}(u_h, v_h)[\psi - \psi_h] \\ =& \sum_{T \in \mathcal{T}_h} \int_T b u_h (\psi - \psi_h) \,\mathrm{d}x \end{aligned}$$

$$
\begin{aligned}
&- \int_T \Big(2 v_h \nabla u_h^\top A_1 \nabla v_h + (v_h^2 + \eta_\varepsilon) \nabla u_h^\top \cdot \operatorname{div}(A_1) \Big) (\psi - \psi_h) \, \mathrm{d}x \\
&+ \int_{\partial T} (v_h^2 + \eta_\varepsilon) \nabla u_h^\top A_1 \, \nu_T \, (\psi - \psi_h) \, \mathrm{d}x \\
= \sum_{T \in \mathcal{T}_h} &\int_T p(u_h, v_h)(\psi - \psi_h) \, \mathrm{d}x + \frac{1}{2} \int_{\partial T} (v_h^2 + \eta_\varepsilon) [\![A_1 \nabla u]\!] \, (\psi - \psi_h) \, \mathrm{d}x
\end{aligned}
$$

Hence, by Hölder's inequality

$$
\begin{aligned}
\big| \partial_u \mathcal{E}(u_h, v_h)[\psi - \psi_h] \big| \leq \sum_{T \in \mathcal{T}_h} &\big\| p(u_h, v_h) \big\|_{L^2(T)} \big\| \psi - \psi_h \big\|_{L^2(T)} \\
&+ \frac{1}{2} \big\| (v_h^2 + \eta_\varepsilon) [\![A_1 \nabla u_h]\!] \big\|_{L^2(\partial T)} \big\| \psi - \psi_h \big\|_{L^2(\partial T)} .
\end{aligned}
$$

So far, $\psi_h \in \mathcal{U}_h$ with $\psi_h = 0$ was chosen arbitrarily. Note, that Q_h is preserving the boundary values so that we can now choose $\psi_h = Q_h \psi$ and infer from Lemma 6.2.1

$$
\begin{aligned}
\big| \partial_u \mathcal{E}_h(u_h, v_h)[\psi - \psi_h] \big| \leq C \sum_{T \in \mathcal{T}_h} &\Bigg(\big\| p(u_h, v_h) \big\|_{L^2(T)} \\
&+ \frac{1}{2\sqrt{\sigma_{T,1} \sigma_{T,2}}} \Big\| \sqrt{h_{\partial T}} (v_h^2 + \eta_\varepsilon) [\![A_1 \nabla u_h]\!] \Big\|_{L^2(\partial T)} \Bigg) \, \| M_T^\top \nabla \psi \|_{L^2(\Delta_T)} ,
\end{aligned}
$$

where we include all the sizes of the reference triangle into the constant C.

Plugging $\psi_h = Q_h \psi$ into the second part of (6.20), and using (6.12) and the fact that $\|\nabla \psi\|_{L^2(\Delta_T)} \leq \frac{1}{\sigma_{T,2}} \| M_T^\top \nabla \psi \|_{L^2(\Delta_T)}$ we achieve

$$
\begin{aligned}
\big| \partial_u \mathcal{E}(u_h, v_h)[\psi_h] \big| &= \big| \partial_u \mathcal{E}(u_h, v_h)[\psi_h] - \partial_u \mathcal{E}_h(u_h, v_h)[\psi_h] \big| \\
&\leq \sum_{T \in \mathcal{T}_h} \Big\| (v_h^2 - \Pi_h(v_h^2)) A_1 \nabla u_h \Big\|_{L^2(T)} \, \| \nabla \psi_h \|_{L^2(T)} \\
&\leq C \sum_{T \in \mathcal{T}_h} \frac{1}{\sigma_{T,2}} \Big\| (v_h^2 - \Pi_h(v_h^2)) A_1 \nabla u_h \Big\|_{L^2(T)} \, \| M_T^\top \nabla \psi \|_{L^2(\Delta_T)} .
\end{aligned}
$$

Together with the former estimate we deduce (6.17).

Let us turn our attention to the second estimator (6.19). For this purpose let $\psi \in H^1(\omega)$, $\psi_h \in \mathcal{V}_h$ with $0 \leq \psi, \psi_h \leq \tilde{v}_h$ and assume that (6.18) holds. Then, we obviously have

$$\begin{aligned}
&\partial_v\mathcal{F}(u_h,v_h)[v_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(v_h-\psi)\,\mathrm{d}x\\
\le{}& \partial_v\mathcal{F}(u_h,v_h)[v_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(v_h-\psi_h)\,\mathrm{d}x\\
&-\partial_v\mathcal{F}_h(u_h,v_h)[v_h-\psi_h]-\frac{\alpha}{\tau}\int_\omega \Pi_h\big((v_h-\tilde v_h)(v_h-\psi)\big)\,\mathrm{d}x\\
\le{}& \partial_v\mathcal{F}(u_h,v_h)[\psi_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(\psi_h-\psi)\,\mathrm{d}x\\
&+\partial_v\mathcal{F}(u_h,v_h)[v_h-\psi_h]-\partial_v\mathcal{F}_h(u_h,v_h)[v_h-\psi_h]\\
&+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(v_h-\psi_h)\,\mathrm{d}x-\frac{\alpha}{\tau}\int_\omega \Pi_h\big((v_h-\tilde v_h)(\psi-v_h)\big)\,\mathrm{d}x\,.
\end{aligned}\tag{6.21}$$

For the first line on the right hand side we get again from the divergence theorem

$$\begin{aligned}
&\partial_v\mathcal{F}_h(u_h,v_h)[\psi_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(\psi_h-\psi)\,\mathrm{d}x\\
={}&\sum_{T\in\mathcal{T}_h}\int_T v_h(\psi_h-\psi)\nabla u_h^\top A_1\nabla u_h\,\mathrm{d}x-\frac{1}{2\varepsilon}\int_T(1-v_h)(\psi_h-\psi)K\,\mathrm{d}x\\
&-2\varepsilon\int_T\nabla v_h\cdot\operatorname{div}(A_2)(\psi_h-\psi)\,\mathrm{d}x+\varepsilon\int_{\partial T}[\![A_2\nabla v_h]\!](\psi_h-\psi)\,\mathrm{d}x\\
&+\frac{\alpha}{\tau}\int_T(v_h-\tilde v_h)(\psi_h-\psi)\,\mathrm{d}x\,,
\end{aligned}$$

and by Hölder's inequality

$$\begin{aligned}
&\left|\partial_v\mathcal{F}_h(u_h,v_h)[\psi_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(\psi_h-\psi)\,\mathrm{d}x\right|\\
\le{}&\sum_{T\in\mathcal{T}_h}\|q(u_h,v_h)\|_{L^2(T)}\|\psi_h-\psi\|_{L^2(T)}+\varepsilon\big\|[\![A_2\nabla v_h^\top]\!]\big\|_{L^2(\partial T)}\big\|\psi_h-\psi\big\|_{L^2(\partial T)}\,.
\end{aligned}$$

As before we choose $\psi_h=Q_h\psi$ and notice that

$$Q_h(\psi-v_h)=\psi_h-v_h\quad\text{and}\quad \psi-\psi_h=\psi-v_h-Q_h(\psi-v_h)\,.$$

Therefore, using (6.13) and (6.14) we obtain

$$\begin{aligned}
&\left|\partial_v\mathcal{F}_h(u_h,v_h)[\psi_h-\psi]+\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(\psi_h-\psi)\,\mathrm{d}x\right|\\
\le{}& C\sum_{T\in\mathcal{T}_h}\Big(\|q(u_h,v_h)\|_{L^2(T)}+\frac{\varepsilon}{\sqrt{\sigma_{T,1}\sigma_{T,2}}}\big\|\sqrt{h_{\partial T}}[\![A_2\nabla v_h^\top]\!]\big\|_{L^2(\partial T)}\Big)\big\|M_T^\top\nabla(\psi-v_h)\big\|_{L^2(\Delta_T)}
\end{aligned}\tag{6.22}$$

Next, we estimate the second line on the right hand side of (6.21) as follows:

$$\partial_v\mathcal{F}(u_h,v_h)[v_h-\psi_h]-\partial_v\mathcal{F}_h(u_h,v_h)[v_h-\psi_h]$$

$$
\begin{aligned}
&= \sum_{T\in\mathcal{T}_h} \int_T (v_h(v_h-\psi_h) - \Pi_h(v_h(v_h-\psi_h)))\nabla u_h^\top A_1 \nabla u_h \,\mathrm{d}x \\
&\quad + \frac{1}{2\varepsilon}\int_T (1-v_h)(v_h-\psi_h) - \Pi_h\big((1-v_h)(v_h-\psi_h)\big)\,\mathrm{d}x\,.
\end{aligned}
$$

Applying Hölder's inequality and the interpolation error estimate from Lemma 6.2.2 we, hence, obtain

$$
\begin{aligned}
&\big|\partial_v\mathcal{F}(u_h,v_h)[v_h-\psi_h] - \partial_v\mathcal{F}_h(u_h,v_h)[v_h-\psi_h]\big| \\
&\le \sum_{T\in\mathcal{T}_h}\left\|\nabla u_h^\top A_1\nabla u_h + \frac{1}{2\varepsilon}K\right\|_{L^2(T)} \big\|v_h(v_h-\psi_h) - \Pi_h\big(v_h(v_h-\psi_h)\big)\big\|_{L^2(T)} \\
&\le C\sum_{T\in\mathcal{T}_h}\frac{h_T^2}{\sigma_{T,2}}\left\|\nabla u_h^\top A_1\nabla u_h + \frac{1}{2\varepsilon}K\right\|_{L^2(T)} |v_h|_{W^{1,\infty}(T)}\big\|M_T^\top\nabla(\psi-v_h)\big\|_{L^2(T)}
\end{aligned}
\tag{6.23}
$$

In the same way we deduce for the third line in (6.21)

$$
\begin{aligned}
&\left|\frac{\alpha}{\tau}\int_\omega (v_h-\tilde v_h)(v_h-\psi_h)\,\mathrm{d}x - \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v_h-\tilde v_h)(v_h-\psi_h)\big)\,\mathrm{d}x\right| \\
&\le \sum_{T\in\mathcal{T}_h}\frac{\alpha}{\tau}|T|^{\frac12}\Big\|(v_h-\tilde v_h)(v_h-\psi_h) - \Pi_h\big((v_h-\tilde v_h)(v_h-\psi_h)\big)\Big\|_{L^2(T)} \\
&\le C\sum_{T\in\mathcal{T}_h}\frac{\alpha\, h_T^2}{\tau\sigma_{T,2}}|T|^{\frac12}|v_h-\tilde v_h|_{W^{1,\infty}(T)}\|M_T^\top\nabla(\psi-v_h)\|_{L^2(T)} \\
&\le C\sum_{T\in\mathcal{T}_h}\frac{\alpha\, h_T^2}{\tau\sigma_{T,2}}\|v_h-\tilde v_h\|_{L^2(T)}\|M_T^\top\nabla(\psi-v_h)\|_{L^2(T)}
\end{aligned}
\tag{6.24}
$$

Adding up (6.22), (6.23) and (6.24) we deduce from (6.21) the requested estimate (6.19), and the proof is complete. □

The estimates of the previous theorem highly depend on the choice of the quasi-interpolation operator. We want to mention that there is another promising quasi-interpolant introduced by Carstensen in [42]. The difference to the operator Q_h is that in general for the interpolation errors (6.11) and (6.12) the patch Δ_T must be extended. In return, however, one can get tighter estimates by replacing $\|p(u_h,v_h)\|_{L^2(T)}$ by $\|p(u_h,v_h)-\overline{p}(u_h,v_h)\|_{L^2(T)}$ in the definition of $\gamma_T(u_h,v_h)$, with $\overline{p}(u_h,v_H)$ being the average of $p(u_h,v_h)$ on T. In a similar way one can exchange $\|q(u_h,v_h)\|_{L^2(T)}$ in the definition of ρ_T. At the end we could not apply this tighter estimates here, since we were not able to implement the required patch for each triangle in the given environment of `FreeFEM` [78]. Nevertheless, from an application point of view the result should not be too different, since a tighter estimate only requires to reduce the error tolerance in order to get the same result. Furthermore, as long as we do not consider the precise value of the constants on the right hand side, the choice of the error tolerance anyway remains based on experience. In order to get an analytical precise error estimate one should additionally compute the constant in the manner of [41]. We keep this idea for future tasks.

As in Remark 6.1.3 we can merge (6.17) and (6.19) to one estimate which is more useful for our mesh adaption procedure. Precisely, (6.16) and (6.18) is equivalent to

$$\partial_u \mathcal{E}_h(u,v)[\psi_{1,h}] + \partial_v \mathcal{F}_h(u,v)[v-\psi_{2,h}] + \frac{\alpha}{\tau}\int_\omega \Pi_h\big((v-v_{i-1})(v-\psi_{2,h})\big)\,\mathrm{d}x \le 0\,,$$

for all $\psi_{1,h} \in \mathcal{U}_h$ with $\psi_1 = 0$ on $\partial\omega$ and for all $\psi_{2,h} \in \mathcal{V}_h$ with $\psi_2 \le v_{i-1}$. This implies now from the just shown theorem that

$$\begin{aligned} &\partial_u \mathcal{E}(u,v)[\psi_1] + \partial_v \mathcal{F}(u,v)[v-\psi_2] + \frac{\alpha}{\tau}\int_\omega (v-v_{i-1})(v-\psi_2)\,\mathrm{d}x \\ &\le C\sum_{T\in\mathcal{T}_h} \gamma_T(u_h,v_h)\|M_T^\top \nabla\psi_1\|_{L^2(\Delta_T)} + \rho_T^{(1)}(u_h,v_h)\big\|M_T^\top \nabla(\psi - v_h)\big\|_{L^2(\Delta_T)}\,, \end{aligned} \tag{6.25}$$

for all $\psi_{1,h} \in \mathcal{U}_h$ with $\psi_1 = 0$ on $\partial\omega$ and for all $\psi_{2,h} \in \mathcal{V}_h$ with $\psi_2 \le v_{i-1}$.

Clearly the anisotropic information is hidden in the matrix $M_T^\top$. In the subsequent section we describe how we extract the necessary information from this estimate in order to construct the new mesh. Beforehand however, we need to make the right hand side of (6.25), which still depends on the test functions ψ_1 and ψ_2, computable. One natural approach would be to deduce some kind of dual norms of the derivatives of $\mathcal{F}(u,v) + \int_\omega (v-v_{i-1})(v-\psi_2)\,\mathrm{d}x$ as it has been done in [39, 40] for an isotropic mesh refinement indicator. Nevertheless, this idea is not expedient when seeking for the anisotropic information. We follow instead the approach from [16] making a specific choice for the test functions: Assuming that we have a critical point $(u,v) \in H^1(\omega)\times H^1(\omega;[0,1])$ with bound $\tilde v_h \in \mathcal{V}_h$, we consider $\varphi = u - u_h$ and $\psi = v$ in (6.25). Neglecting the constant, we can thus estimate the right hand side of (6.25) by

$$\Xi(u_h,v_h) := \sum_{T\in\mathcal{T}_h} \Xi_T(u_h,v_h)$$

where we set for all $T\in\mathcal{T}_h$

$$\begin{aligned} \Xi_T(u_h,v_h) := \gamma_T(u_h,v_h)&\|M_T^\top\nabla(u-u_h)\|_{L^2(\Delta_T)} \\ &+ \rho_T(u_h,v_h)\big\|M_T^\top\nabla(v-v_h)\big\|_{L^2(\Delta_T)}\,. \end{aligned} \tag{6.26}$$

Approximating the first-order derivatives of $u-u_h$ and $v-v_h$ by Zienkiewicz–Zhu recovery procedure, as detailed in [59], the size $\Xi(u_h,v_h)$ is now computable. In the next section we show how we iteratievly construct a new mesh from the information provided by $\Xi(u_h,v_h)$ computed on the old mesh. We follow the general strategy to find the mesh with a minimum of triangles such that $\Xi(u_h,v_h)$ is smaller than a certain tolerance, say `TOL` > 0. To do this we equally distribute this error tolerance on all triangles of the triangulation $\mathcal{T}_h$. Hence, we require

$$\Xi_T(u_h,v_h) \le \frac{\texttt{TOL}}{\#\mathcal{T}_h} \quad \text{for all } T\in\mathcal{T}_h\,.$$

6.3 Construction of the Mesh

For the construction of the new mesh out of the information gained by Ξ we follow the strategy from [16, 66, 92] of a metric based mesh creation. Fixing a reference triangle one can couple a unique metric to every arbitrary triangle. At the beginning of the previous section we considered for each $T \in \mathcal{T}_h$ the affine function that maps the reference triangle onto T, whose linear part was described by the matrix $M_T = U_T \Sigma_T V_T^\top$. Here, the right hand side is the singular value decomposition, where we pursue the convention that the diagonal entries $\sigma_{T,1}, \sigma_{T,2}$ of Σ_T are ordered in size. Thus, we assume $\sigma_{T,1} \geq \sigma_{T,2}$. Since U and V are orthogonal we can actually write $M_T = U_T \Sigma_T U_T^\top R_T$ with $R_T = U_T V_T^\top$ being again orthogonal. The matrix $\widetilde{M}_T = U_T \Sigma_T U_T^\top$ is now positive definite and symmetric, thus it defines a metric on T. Note that with respect to this metric, every triangle is uniform, i.e. $\sqrt{\vec{e}^\top \widetilde{M}_T \vec{e}} = 1$ for all edge-vectors $\vec{e}$ of T. For the given mesh $\mathcal{T}_h$ we can define in this way a whole metric field $\mathcal{M} \colon \omega \to \mathbb{R}^{2\times 2}$ given by $\mathcal{M} = \widetilde{M}_T$ on $T \in \mathcal{T}_h$.

The key to our mesh construction is that the whole procedure can be turned around in the sense that for a given metric field $\mathcal{M} \colon \omega \to \mathbb{R}^{2\times 2}$ we can construct a corresponding mesh, whose triangles are associated as close as possible to this metric. This is done by the Delaunay algorithm taking care of this metric. Usually, a Delaunay triangulation provides a uniform isometric mesh with almost uniform triangles. One can perform the algorithm constructing a triangulation which is uniform with respect to a specific metric which results in the required anisotropic mesh in the Euclidean space. Details for the mechanism of the Delaunay triangulation can be found, for instance, in [44, 74]. For us, at this point, it is enough to know that the finite element tool `FreeFEM` [78], which we are going to use for our simulations, provides the function `adaptmesh`, which does exactly the job for us. Thus our goal is now to find the right metric field for the new mesh. We therefore assume that a triangulation $\mathcal{T}_h^{(j)}$ is given for some $j \in \mathbb{N} \cap \{0\}$. We then compute a metric field on that mesh which is used for constructing a posteriori a new mesh $\mathcal{T}_h^{(j+1)}$. For this purpose, we have a closer look on the different sizes M_T, $\sigma_{T,i}$, etc. which we suppose to be associated to the preexisting triangulation $T \in \mathcal{T}_h^{(i)}$.

For $T \in \mathcal{T}_h^{(i)}$ the metric is characterized by the singular values $\sigma_{T,1}$, $\sigma_{T,2}$ and the corresponding singular vectors $\mathbf{r}_{T,1}$ respectively $\mathbf{r}_{T,2}$, which are the column vectors of U_T. We refer again to Figure 6.1 for a geometric illustration. We remark that by knowing one of the two singular vectors, say $\mathbf{r}_{T,1}$, we can reconstruct $\mathbf{r}_{T,2}$ by an orthonormal basis completion.

Using the fact that $M_T^\top = V_T \Sigma_T U_T^\top$ and that V_T is orthogonal we can compute in this setting (like in [65])

$$\begin{aligned}\|M_T^\top \nabla\psi\|^2_{L^2(\Delta_T)} &= \|\Sigma_T U_T^\top \nabla\psi\|^2_{L^2(\Delta_T)}\\ &= \sum_i \int_{\Delta_T} \sigma_{T,i}^2 |\mathbf{r}_{T,i}\cdot\nabla\psi|^2 \,\mathrm{d}x\\ &= \sum_i \sigma_{T,i}^2\, \mathbf{r}_{T,i}^\top\, G_T(\psi)\, \mathbf{r}_{T,i}\,.\end{aligned}$$

for all $\mathcal{T}\in\mathcal{T}_h^{(i)}$ and for all $\psi\in H^1(\omega)$. For all $T\in\mathcal{T}_h^{(i)}$ we have set here $G_T\colon H^1(\Delta_T)\mapsto L^2(\Delta_T;\mathbb{R}^{2\times2})$ defined by

$$G_T(\psi) = \begin{pmatrix} \displaystyle\int_{\Delta_T} |\partial_1\psi|^2\,\mathrm{d}x & \displaystyle\int_{\Delta_T} \partial_1\psi\,\partial_2\psi\,\mathrm{d}x \\ \displaystyle\int_{\Delta_T} \partial_1\psi\,\partial_2\psi\,\mathrm{d}x & \displaystyle\int_{\Delta_T} |\partial_2\psi|^2\,\mathrm{d}x \end{pmatrix} \quad \text{for all } \psi\in H^1(\Delta_T)\,.$$

In this way we make the anisotropic information, which was hidden in M_T, visible. From (6.26) we hence obtain

$$\begin{aligned}\Xi_T(u_h,v_h) := \gamma_T(u_h,v_h)\Big(\sum_i \sigma_{T,i}^2\,\mathbf{r}_{T,i}^\top\, G_T(u_h)\,\mathbf{r}_{T,i}\Big)^{\frac12}&\\ + \rho_T(u_h,v_h)\Big(\sum_i \sigma_{T,i}^2\,\mathbf{r}_{T,i}^\top\, G_T(v_h)\,\mathbf{r}_{T,i}\Big)^{\frac12}&\,.\end{aligned}$$

Instead of $\sigma_{T,1}$ and $\sigma_{T,2}$ for $T\in\mathcal{T}_h^{(i)}$ we consider the triangle area size which is $|T| = |\hat{T}|\sigma_{T,1}\sigma_{T,2}$ and the ratio $s_T := \frac{\sigma_{T,1}}{\sigma_{T,2}}$ which describes the stretching of the triangle and thus measures its anisotropy. Note, that we always have $s_T\geq 1$, and the larger s_T the more anisotropic the corresponding triangle is. In fact for $s_T = 1$ the triangle is uniform. We call s_T also the *stretching factor* of T. We can now gather all the information about the area of T by factorization as follows

$$\Xi_T(u_h,v_h) = \alpha_T\,\Upsilon_T(s_T,\mathbf{r}_{T,1}) \quad \text{for all } T\in\mathcal{T}_h^{(i)}\,,$$

with the following definitions

$$\begin{aligned}\alpha_T &:= |\hat{T}|(\sigma_{T,1}\,\sigma_{T,2})^{\frac32}\\ \Upsilon_T(s_T,\mathbf{r}_{T,1}) &:= \Big(s_T\,\mathbf{r}_{T,1}^\top\,\Gamma_T(u_h,v_h)\,\mathbf{r}_{T,1} + \frac{1}{s_T}\,\mathbf{r}_{T,2}^\top\,\Gamma_T(u_h,v_h)\,\mathbf{r}_{T,2}\Big)^{\frac12}\,,\\ \Gamma_T(u_h,v_h) &:= \overline{\gamma}_T^2(u_h,v_h)\,\overline{G}_T(u_h) + \overline{\rho}_T^2(u_h,v_h)\,\overline{G}_T(v_h)\,,\\ \overline{\gamma}_T(u_h,v_h) &:= \frac{\gamma_T(u_h,v_h)}{|T|^{\frac12}} \quad \text{and} \quad \overline{\rho}_T(u_h,v_h) := \frac{\rho_T(u_h,v_h)}{|T|^{\frac12}}\,,\end{aligned}$$

$$\overline{G}_T(\psi) := \frac{G_T(\psi)}{|\hat{T}|\sigma_{T,1}\sigma_{T,2}} \quad \text{for all } \psi \in H^1(\Delta_T)\,.$$

The idea behind these choices is that $\overline{\gamma}_T(u_h, v_h)$, $\overline{\rho}_T(u_h, v_h)$ and $\overline{G}_T(\cdot)$, which are mainly L^2-norms are now averaged over T, so that in the limit as the mesh becomes finer and finer, we have some approximately pointwise values here. All the required information are therefore solely retained in α_T and $\Upsilon_T(s_T, \mathbf{r}_{T,1})$, where α_T gathers all information about the area of T and $\Upsilon_T(s_T, \mathbf{r}_{T,1})$ only depends on the stretching factor s_T and the vector $\mathbf{r}_{T,1}$. Once u_h, v_h is fixed on $\mathcal{T}_h^{(j)}$ they are not of interest any more, which is the reason why we do not write their dependency for Υ_T anymore.

Equivalently to finding the mesh with the least number of triangles for which holds $\Xi_T(u_h, v_h) \leq \frac{\mathtt{TOL}}{\#\mathcal{T}_h^{(i)}}$ for all $T \in \mathcal{T}_h^{(i)}$, we now minimize $\Upsilon_T(s_T, \mathbf{r}_{T,1})$ with respect to $s_T > 0$ and $\mathbf{r}_{T,1} \in \mathbb{S}^1$ in order to choose the area of K, respectively α_K, as large as possible. Fortunately, the minimization of $\Upsilon_T(s_T, \mathbf{r}_{T,1})$ can be solved analytically (see [67, Proposition 14]). For $\mathbf{v}_{T,i}, \vartheta_{T,i}$ being the eigenvector-eigenvalue pair of $\Gamma_T(u_h, v_h)$ for $i = 1, 2$ with $\vartheta_{T,1} > \vartheta_{T,2}$, we have

$$\sqrt{2}\,(\vartheta_{T,1}\,\vartheta_{T,2})^{\frac{1}{4}} = \Upsilon_T(\widetilde{s}_T, \mathbf{v}_{T,2}) = \min_{s_T>0,\, \mathbf{r}_{T,1}\in\mathbb{S}^1} \Upsilon_T(s_T, \mathbf{r}_{T,1})\,.$$

with $\widetilde{s}_T = \sqrt{\frac{\vartheta_{T,1}}{\vartheta_{T,2}}}$. In order to obtain the singular values $\sigma_{T,1}$ and $\sigma_{T,2}$ for the metric field associated to the new mesh $\mathcal{T}_h^{(i+1)}$ we, therefore, solve on each $T \in \mathcal{T}_h^{(i)}$ the following system of equations

$$\frac{\sigma_{T,1}}{\sigma_{T,2}} = s_T = \sqrt{\frac{\vartheta_{T,1}}{\vartheta_{T,2}}} \quad \text{and} \quad \alpha_T\sqrt{2}(\vartheta_{T,1}\,\vartheta_{T,2})^{\frac{1}{4}} = \frac{\mathtt{TOL}}{\#\mathcal{T}_h^{(i)}}\,.$$

Using $\alpha_T = |\hat{T}|(\sigma_{T,1}\sigma_{T,2})^{\frac{3}{2}}$ we, hence, obtain the following distinct values

$$\sigma_{T,1} = \left(\frac{\mathtt{TOL}}{\sqrt{2}\,|\hat{T}|\,\#\mathcal{T}_h^{(i)}}\,\frac{\sqrt{\vartheta_{T,1}}}{\vartheta_{T,2}}\right)^{\frac{1}{3}} \quad \text{and} \quad \sigma_{T,2} = \left(\frac{\mathtt{TOL}}{\sqrt{2}\,|\hat{T}|\,\#\mathcal{T}_h^{(i)}}\,\frac{\sqrt{\vartheta_{T,2}}}{\vartheta_{T,1}}\right)^{\frac{1}{3}}. \qquad (6.27)$$

The singular vectors are obtained by setting $\mathbf{r}_{T,1} = \mathbf{v}_{T,2}$ and choosing $\mathbf{r}_{T,2} \in \mathbb{S}^1$ such that $\mathbf{r}_{T,1} \cdot \mathbf{r}_{T,2} = 0$. In this way we obtain the new metric field $\mathcal{M}^{(i+1)}$ that is piecewise constant on the old mesh $\mathcal{T}_h^{(i)}$. By the Delaunay triangulation algorithm we can then construct the new mesh $\mathcal{T}_h^{(i+1)}$ based on this metric.

The description of the complete algorithm that is computed together with some numerical examples are presented in the next section.

6.4 Numerical Examples

Before we compute some concrete examples we need to describe how to perform the mesh adaption within the scheme (6.5)–(6.6). In [16] the authors propose two algorithms.

In the first one they adapt the mesh after the alternation terminated. In the second algorithm the new mesh is computed within each of the alternating steps. The last approach turned out to provide better results when considering the crack path; however, it is computational much more expensive since the many mesh adaptions take rather much time. For this reason we will pursue a compromise of those tow algorithms, in which we regularly adapt the mesh after a certain number of alternating minimizations. We sho the details in Algorithm 6.1. Note, that we stop the whole iteration when the change of the phase field variable is below a certain threshold, called $\texttt{TOL}_v$ and the numbers of nodes does not change significantly when passing from the old to the new mesh. Each time after creating a new mesh, we need to interpolate our functions on the new finite element space created by the new mesh, which is done by the standard Lagrange interpolator. We write $\Pi_h^{(j)}$ for the interpolation operator on the mesh $\mathcal{T}_h^{(j)}$. The constraint minimization of the phase field variable is solved by an interior point method using the package `Ipopt` [105] which can be easily included in `FreeFEM` [78].

In order to implement our fracture phase field model from Section 4.2 we have to set $A_1 = \mu(a^{\alpha\beta})\sqrt{a}$, $A_2 = (a^{\alpha\beta})\sqrt{a}$, $K = \kappa\sqrt{a}$ and $b = \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau}$ with the notation of Chapter 3, where $(a^{\alpha\beta})$ is the contravariant metric tensor $b_{\alpha\beta}$ the curvature and $\boldsymbol{c}^{\alpha\beta\sigma\tau} = \frac{2\lambda\mu}{\lambda+2\mu} a^{\alpha\beta} a^{\sigma\tau} + \mu(a^{\alpha\sigma}a^{\beta\tau} + a^{\alpha\tau}a^{\beta\sigma})$ the two-dimensional stiffness tensor and κ the constant toughness of the material. During the following simulations we set all the parameters and tolerances appearing in the energy functional and in Algorithm 6.1 to the values in Table 6.1 as long as not stated differently.

The implementation of an initial crack is done by cutting a thin slit out of the domain. This idea goes back to [27] and has been used in all the simulations that we know from the literature. Although the approach of choosing an initial phase field for the crack initialization, as we did in Section 5.5, would be closer to the theory of time evolution, we save a lot of computation time in initializing the crack by a slit. Furthermore, to be honest, the phase field initialization does not work very well with our anisotropic mesh adaption procedure for reasons we do not understand yet.

The time dependent boundary condition which we impose for the displacement field is chosen linearly in time. For technical reasons we have to extend the physical domain beyond the Dirichlet boundary condition,. This is due to the fact that we are originally approximate the Mumford-Shah-like functional due to some boundary value problem on the function space $\mathrm{GSBV}(\omega)$. In order to allow jumps along the Dirichlet boundary condition, one needs to consider extended domains on such function spaces. Also for the phase field model such an extension is reasonable, because otherwise when breaking close to the Dirichlet boundary not the full thickness of the phase field is visible, so that the energy would be underestimated. For the results of our computations below we do not visualize this extension of the domain since it is not physically existing.

A Piece of the Cylinder

We start with a fracture simulation of a part of a cylindrical surface with radius $R > 0$ and length $L > 0$. As a diffeomorphism we naturally choose cylindrical coordinates.

Algorithm 6.1 Alternating Minimization including Anisotropic Mesh Adaption

initialize $v_0, u_0, \mathcal{T}_h^{(0)}$
for $i = 0$ to k **do**
    $j, l \leftarrow 0$
    $u_{i,0} \leftarrow u_0$
    $v_{i,0} \leftarrow v_0$
    repeat
        $m \leftarrow 0$
        $l \leftarrow l + 1$
        repeat
            $j \leftarrow j + 1$
            $m \leftarrow m + 1$
            $u_{i,j} \leftarrow \arg\min\{\mathcal{E}_h(u, v_{i,j-1}) : u \in \mathcal{U}_h, u = g(t_i) \text{ on } \partial\omega\}$
            $v_{i,j} \leftarrow \arg\min\left\{\mathcal{F}_h(u_{i,j}, v) + \frac{\alpha}{\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h, v \leq v_{i-1}\right\}$
        until $m = \texttt{MaxIt}$ **or** $\|v_{i,j} - v_{i,j-1}\|_\infty < \texttt{TOL}_v$
        compute the new metric field $\mathcal{M}^{(m+1)}$ based on (6.27) with $u_h = u_{i,j}$, $v_h = v_{i,j}$ and $\texttt{TOL} = \texttt{TOL}_{\text{ref}}$.
        create the new mesh $\mathcal{T}_h^{(m+1)}$ associated to the metric $\mathcal{M}^{(m+1)}$
        $v_{i,j} \leftarrow \Pi_h^{(m+1)}(v_{i,j})$
    until $\frac{|\#\mathcal{T}_h^{(j+1)} - \#\mathcal{T}_h^{(j)}|}{\#\mathcal{T}_h^{(j)}} < \texttt{TOL}_{\text{mesh}}$ **and** $\|v_{i,j} - v_{i,j-1}\|_\infty < \texttt{TOL}_v$
    $v_i \leftarrow \arg\min\left\{\mathcal{F}_h(u_{i,j}, v) + \frac{\alpha}{\tau}\|v - v_{i-1}\|^2_{\mathcal{V}_h} : v \in \mathcal{V}_h, v \leq v_{i-1}\right\}$
    $u_i \leftarrow \arg\min\{\mathcal{E}_h(u, v_{i,j-1}) : u \in \mathcal{U}_h, u = g(t_i) \text{ on } \partial\omega\}$
    $\mathcal{T}_h^{(0)} = \mathcal{T}_h^{(j)}$
end for

Table 6.1: Chosen values for the parameters and tolerances appearing in Algorithm 6.1.

$\texttt{TOL}_{\text{ref}}$	$\texttt{TOL}_{\text{mesh}}$	$\texttt{TOL}_v$	$\texttt{MaxIt}$	τ	ε	η	κ	λ	μ
10^{-3}	10^{-2}	$2 \cdot 10^{-3}$	8	10^{-2}	$5 \cdot 10^{-3}$	10^{-5}	1	0	1

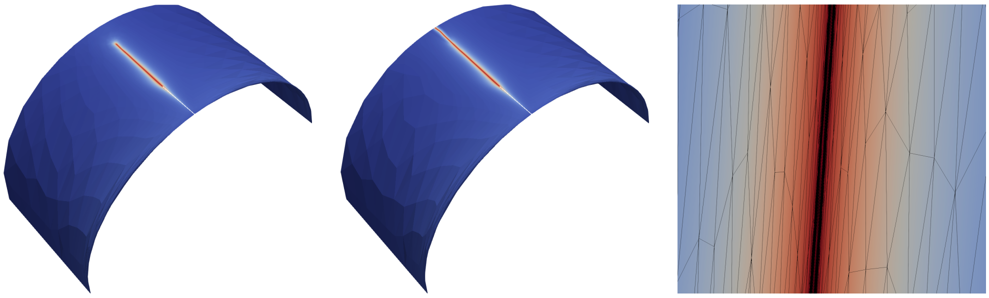


Figure 6.2: Phase Field of a crack Simulation of a cylinder with boundary condition g_1 at different times.

Particularly, we consider the following parametrization:

$$(x, y) \mapsto \begin{pmatrix} R\cos x \\ R\sin x \\ y \end{pmatrix} \quad \text{for all } (x, y) \in \omega = \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \times (0, L)\,.$$

With this at hand we have

$$(a^{\alpha\beta}) = \begin{pmatrix} \frac{1}{R^2} & 0 \\ 0 & 1 \end{pmatrix}, \quad (b_{\alpha\beta}) = \begin{pmatrix} -R & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \sqrt{a} = R\,.$$

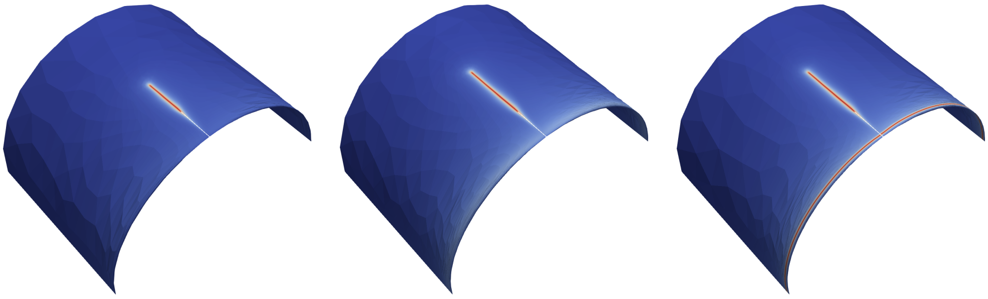
For the crack initialization we define the pre-crack $\Gamma_1 = [-10^{-3}, 10^{-3}] \times [0, 0.3]$. Hence, the computation takes place on $\omega \setminus \Gamma_1$. The boundary condition is imposed on the boundary where the crack starts. Precisely, we set

$$g_1(t) = \begin{cases} t & \text{on } \left[10^{-3}, \frac{\pi}{2}\right] \times \{0\} \\ -t & \text{on } \left[-\frac{\pi}{2}, -10^{-3}\right] \times \{0\}\,. \end{cases}$$

As explained above for the computations we actually work on the extended domain $\omega \cup (-\frac{\pi}{2}, \frac{\pi}{2}) \times (-0.1, 0]$ deleting the extension afterwards for visualization as it is not of physical presence. Furthermore, we consider the image of ω provided by the parametrization above in order to see the actual cylindrical surface.

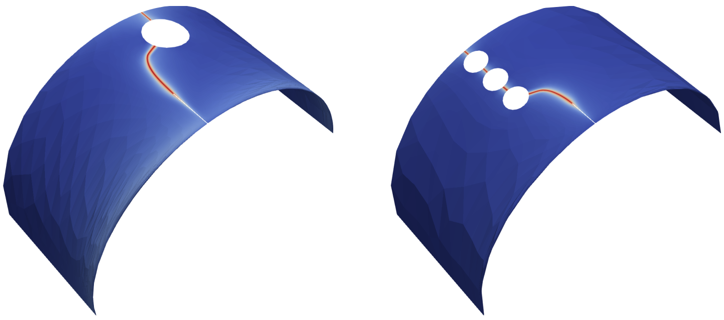
For now, we set in the given examples $R = 1$. In Figure 6.2 we can see the phase field computed for $L = 1$ as well as an enlargement of the mesh close to the crack. One can see that the mesh is well aligned along the crack, which shows the advantage of taking the anisotropy into account.

Note that the term $\int_\omega \boldsymbol{c}^{\alpha\beta\sigma\tau} b_{\alpha\beta} b_{\sigma\tau} |u|^2 \sqrt{a}\,\mathrm{d}x$ in the functional counts some energy even if the displacement is constant. This leads to some effect that does not appear in the anti-planar setting. The boundary condition creates some tension along the boundary. Thus, if the length L is chosen too large a crack appears along the boundary



$t = 1.91$ $t = 2.83$ $t = 2.84$

Figure 6.3: Phase Field of a crack Simulation of a cylinder with boundary condition g_1 and $L = 2$ at different times.

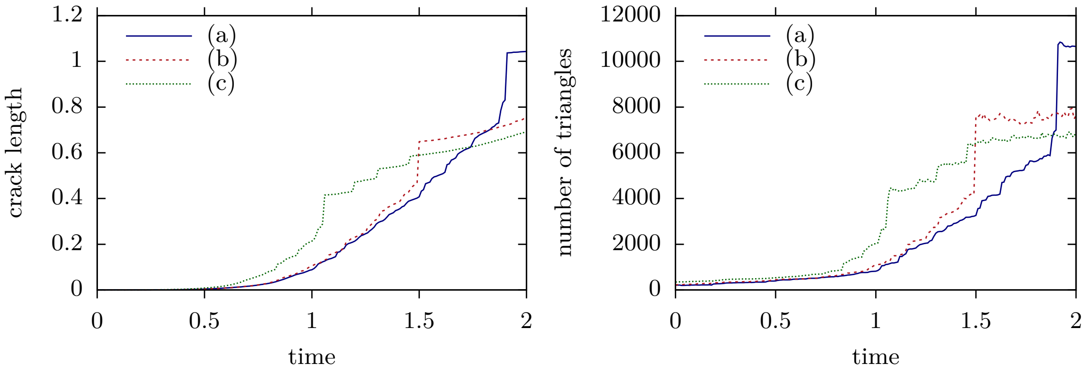


Single hole at time $t = 2.97$ Three holes at time $t = 1.46$

Figure 6.4: Final phase fields of a crack Simulation of a cylinder with boundary condition g_1 and $L = 1$ at different times.

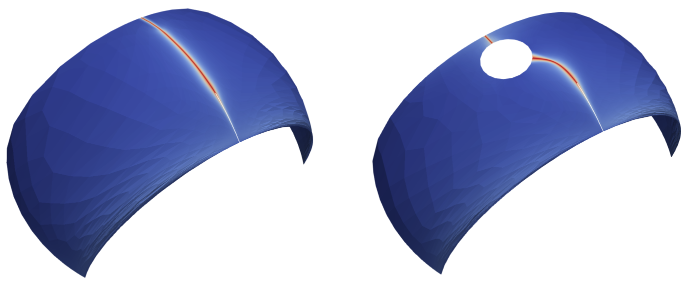
before it is completed in the direction of initial crack. Indeed this phenomenon can be observed in Figure 6.3 where we choose $L = 2$. The crack continues propagating at time $t = 1.91$, where the crack of the shorter cylinder was completed, until $t = 2.83$. Then, the surface suddenly breaks along the Dirichlet boundary at time $t = 2.84$. In order to keep the responsible term as small as possible we choose $\lambda = 0$ in all the examples.

Inspired from the examples in the anti-planar setting in [16, 38], we present another simulation in Figure 6.4, cutting holes into the domain in order to influence the crack path. The single hole is centered at $(0.3, 0.75)$ and has radius 0.15. The radius of the the three holes is 0.08 and their centers are located at $(-0.2, 0.88)$, $(-0.2, 0.68)$ and $(-0.2, 0.48)$. To give more detailed information we plot for some of the examples the number of triangles and the crack length at each time step in Figure 6.5. The crack length is computed by $\frac{1}{\kappa}\mathcal{D}_h(v)$ since this part Γ-convergence to the length of the crack (see Remark 4.2.1). It is not surprising that the number of triangles grows with the length of the crack, since the area where the phase field has a large gradient correlates to the crack length.



Crack length   Number of triangles

Figure 6.5: Crack length and the number of triangles forming the mesh as functions of time. Function (a) corresponds to the plain cylinder; function (b) belongs to the cylinder with one hole, and function (c) to the one with three holes.



$\bar{y} = \frac{\pi}{6}$, $t = 2.38$ $\bar{y} = \frac{\pi}{7}$, $t = 2.64$

Figure 6.6: Final phase fields of a crack Simulation of a part of a spherical surface with boundary condition g_1, with and without a hole in the domain.

A Piece of the Sphere

As another example we consider a small part of a sphere with radius $R > 0$. We use the parametrization

$$(x, y) \to R \begin{pmatrix} \cos(x)\cos(y) \\ \sin(x)\cos(y) \\ \sin(y) \end{pmatrix} \quad \text{for } (x, y) \in \omega := (-\bar{x}, \bar{x}) \times (-\bar{y}, \bar{y})$$

for some $0 < \bar{x} < \pi, 0 < \bar{y} < \frac{\pi}{2}$. With this setting we have

$$(a^{\alpha\beta}) = \begin{pmatrix} \frac{1}{R^2\cos^2(y)} & 0 \\ 0 & \frac{1}{R^2} \end{pmatrix}, \quad (b_{\alpha\beta}) = \begin{pmatrix} -R\cos^2(y) & 0 \\ 0 & -R \end{pmatrix} \quad \text{and} \quad \sqrt{a} = R^2\cos(y)\,.$$

For simplicity we set again $R = 1$ and $\bar{x} = \frac{\pi}{2}$. Changing the radius does not result in significantly different results. The pre-crack is set to $\Gamma_2 = [-10^{-3}, 10^{-3}] \times [-\bar{y}, 0.3 - \bar{y}]$

and for the boundary condition we again choose g_1 from above. Figure 6.6 shows the phase field for two different settings with domain $\omega \setminus \Gamma_2$, where again in one example a hole is cut to the domain with center $(-0.25, 0.5)$ and radius 0.15. Choosing $\bar{y}$ smaller when the hole is added, is due to the fact that otherwise the surface again breaks along the Dirichlet boundary.

We close this chapter with a kind of smart presentation of the fracture simulation. In Figure 6.7 we plot the deformed specimen for many different time steps. Beforehand we cut out the nodes of the mesh, where the phase field variable is below a certain tolerance, whose value is chosen to be 10^{-2}. In this way we identify the position of the crack and the surface looks really broken.

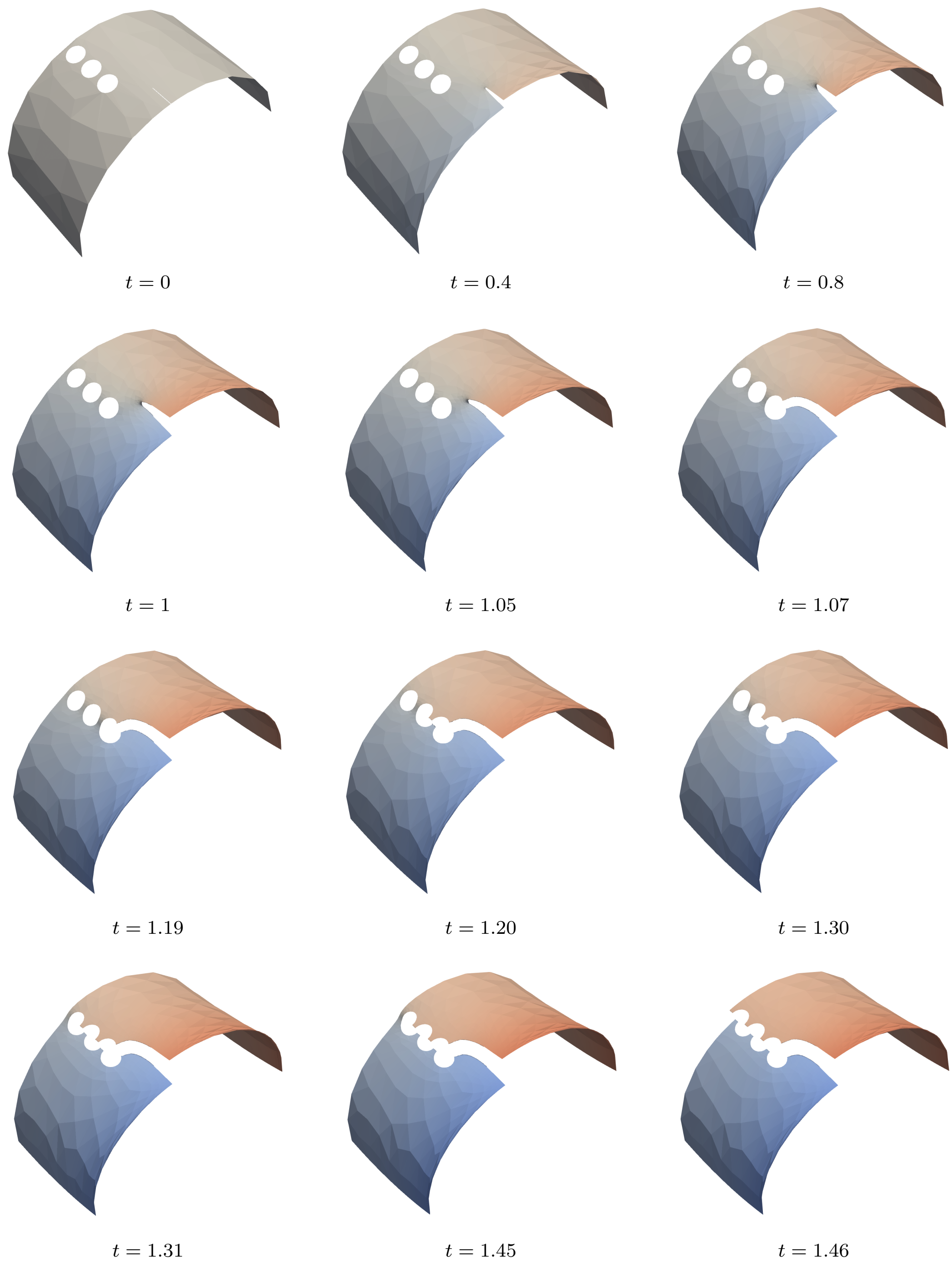


Figure 6.7: Deformed cylinder with three holes at different times with the nodes along the detected crack being removed.

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