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Abstract. An adaptive finite element semi-smooth Newton solver for the Cahn-Hilliard model with double obstacle free energy is proposed. For this purpose, the governing system is discretised in time using a semi-implicit scheme, and the resulting time-discrete system is formulated as an optimal control problem with pointwise constraints on the control. For the numerical solution of the optimal control problem, we propose a function space based algorithm which combines a Moreau-Yosida regularization technique for handling the control constraints with a semi-smooth-Newton method for solving the optimality systems of the resulting sub-problems. Further, for the discretization in space and in connection with the proposed algorithm, an adaptive finite element method is considered. The performance of the overall algorithm is illustrated by numerical experiments.

1. Introduction

The mathematical study of interface dynamics has attracted a lot of interest in the last decades. Applications include multi-phase flow, crack propagation, solidification, melting processes, lubrication mechanisms, etc. [10]. Two major approaches have been used for tracking interfaces: sharp interface models and phase-field models, respectively. In the former, the interface is described as an evolving manifold whose motion is controlled by boundary conditions which are consistent with the physics of the modeled mechanism. In phase-field approaches an additional order parameter is introduced, which is continuous in space but preferably takes distinct constant values in each phase. As a consequence, the physical interface is located in the transition zone where this parameter changes its value. By driving the thickness of the transition zone to zero, typically the sharp-interface limit is obtained. Mathematically, phase-field models convert a free-boundary problem into a set of partial differential equations which allow for a more convenient numerical treatment.

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A typical phase-field model which has proven to be excellent for describing several physical phenomena such as, e.g., phase transitions in binary alloys is given by the Cahn-Hilliard system [8]. It was originally derived for spinodal decomposition occurring when a homogeneous high-temperature mixture of two metallic components is rapidly quenched below a critical temperature. The mixture becomes inhomogeneous and forms a structure alternating between the two alloy components. Later, the Cahn-Hilliard theory was adopted to a broad range of applications exhibiting similar phase separation behavior. Examples include problems in mathematical image processing [15], in fluid dynamics [1] or even in cancer growth modeling [20].

Based on minimizing an energy functional of Ginzburg-Landau type, the Cahn-Hilliard model gives rise to a mathematical system involving a parabolic forth order (in space) operator. A mixed formulation splits this operator into a coupled parabolic-elliptic second order (in space) system. Depending on the underlying free energy, a variational inequality might occur. The latter is in particular true for the popular double obstacle free energy, which was thoroughly analyzed by Blowey and Elliot in [6]. In [7] the same authors investigated the problem from a numerical point of view. Concerning the efficient algorithmic treatment of Cahn-Hilliard models involving the double obstacle potential we mention here the preconditioned Uzawa type solver proposed recently by Gräser and Kornhuber [22] and the many references therein. Based on this algorithm, an adaptive finite element solver was designed and applied successfully to problems in two and three spatial dimensions in [3] and [4].

The aim of the present paper is to supplement existing algorithmic approaches like the one in [22] for solving the Cahn-Hilliard model with double obstacle potential. The proposed method is of semi-smooth Newton type and allows for a convergence analysis in function space. In view of the theory in [26], one then expects a mesh-independent behavior of the algorithm, i.e. once the discretization is "fine" enough the convergence rate of the discrete scheme matches the one of its continuous counterpart. In particular, further mesh refinements should not adversely affect the convergence behavior of the discretized method. For the discretization in time we use a semi-implicit scheme, and, following [21, 22] and the references therein, we formulate the time-discrete system as an optimal control problem with pointwise constraints on the control. The constraints are handled by a regularization of Moreau-Yosida type which is related to an augmented Lagrangian penalization. The optimality systems of the resulting regularized (sub-)problems are solved by a local superlinearly convergent semi-smooth-Newton method [23]. Within the framework considered in this paper, the solution at a given time provides an excellent initial point for the semi-smooth-Newton method for computing the solution at the next time step. We recall that usually the time step size is related to the interface width due to the phase-field approach. The good initial guess enables one even to operate with little regularization, i.e. large penalty parameter, without suffering from ill-conditioning or mesh-dependence effects. In order to further enhance the efficiency of our algorithm, we explore an adaptive finite element method for the discretization in space utilizing a posteriori techniques. In the discrete setting and in connection with the semi-smooth Newton method, we also show that the resulting linear systems are well posed and are solved efficiently by using Schur complements.

The rest of this paper is organized as follows. In Section 2 we describe the Cahn-Hilliard model with the double obstacle free energy. In section 3 a semi-implicit time discrete problem is considered. We show that the time-discrete problem is equivalent to an optimal control problem whose regularized version is introduced and analyzed in section 4. In section 5 we propose a semi-smooth Newton method to solve the regularized sub-problems. In section 6 we design an adaptive finite element algorithm based on a posteriori error analysis. Finally, numerical experiments are reported on in section 7.

2. Cahn-Hilliard model

For time $t \in (0,T)$, with $T > 0$ fixed, we consider an alloy composed of a binary mixture of components A and B with respective concentrations c_A and c_B located in the spatial domain $\Omega \subset \mathbb{R}^n$ with $n \in \{1,2,3\}$. The local phase variable

$$u = \frac{c_A - c_B}{c_A + c_B} \quad \text{in } \Omega,$$

satisfies $-1 \leq u \leq 1$ with $u \equiv 1$ ($u \equiv -1$) in the pure B-phase (A-phase) region. A mixture of the two components yields $-1 < u < 1$ and gives rise to an interfacial layer. Following [19], under mass conservation the equilibrium profile of the mixture minimizes the Ginzburg-Landau energy

$$\mathcal{E}_\gamma(u) = \frac{\gamma}{2}\int_\Omega |\nabla u|^2 dx + \int_\Omega \Psi(u) dx.$$

Here, $\sqrt{\gamma}$ relates to the width of the interface region and $\Psi(u)$ denotes the homogeneous free-energy density. The generalized chemical potential w is given by

$$w := \frac{\delta \mathcal{E}_\gamma}{\delta u} = -\gamma \Delta u + \Psi'(u), \tag{2.1}$$

and mass conservation (see [8]) yields

$$\frac{\partial u}{\partial t} = -\nabla \cdot \boldsymbol{J} \quad \text{with } \boldsymbol{J} = -M(u)\nabla w, \tag{2.2}$$

where $M(u)$ is the mobility. Degenerate mobilities can be motivated by practical applications and were considered, e.g. in [5, 18]. In this paper, however, we assume a non-degnerate case and use, without loss of generality, $M(u) \equiv 1$. It is well-known that the equations (2.1) and (2.2) constitute the Cahn-Hilliard system.

Concerning the free energy Ψ, besides the double-well and logarithmic potentials considered in the literature (see for instance [17, 13]), the double-obstacle potential is a good approximation in particular for deep quenches [7]. It is given by

$$\Psi(u) := \begin{cases} \frac{1}{2}(1-u^2) & \text{if } u \in [-1,1], \\ +\infty & \text{if } u \notin [-1,1]. \end{cases}$$

In this case, (2.1) becomes

$$w + \gamma\Delta u \in \partial\Psi(u), \tag{2.3}$$

where $\partial\Psi$ is the subdifferential of Ψ. The potential equation (2.3) is equivalent to

$$|u| \le 1, \quad \langle -\gamma\Delta u - w - u, v - u\rangle \ge 0 \quad \forall v \text{ with } |v| \le 1. \tag{2.4}$$

We supplement (2.2) and (2.4) by appropriate initial and boundary conditions:

$$u_0 \in \mathcal{K} := \left\{ v \in H^1(\Omega) : |v| \le 1 \text{ in } \Omega \right\}, \quad \frac{\partial w}{\partial \boldsymbol{n}} = \frac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \partial\Omega,$$

respectively. Summarizing, the variational form of our Cahn-Hilliard system with a constant mobility and the double obstacle free energy consists in finding the order parameter u and the chemical potential w such that

$$(u,w) \in H^1(0,T,H^1(\Omega)) \cap L^\infty(0,T,H^1(\Omega)^*) \times L^2(0,T,H^1(\Omega)), \tag{2.5}$$

$$u(t) \in \mathcal{K} \qquad \forall t \in]0,T[, \tag{2.6}$$

$$\left\langle \frac{\partial u}{\partial t}, v \right\rangle + (\nabla w, \nabla v) = 0, \quad \forall v \in H^1(\Omega), \tag{2.7}$$

$$\gamma(\nabla u, \nabla v - \nabla u) - (u, v-u) \ge (w, v-u) \quad \forall v \in \mathcal{K}, \tag{2.8}$$

$$u(0) = u_0, \tag{2.9}$$

where $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle$ stand for the usual $L^2(\Omega)$-inner product and the duality pairing of $H^1(\Omega)$ and its dual $H^1(\Omega)^*$, respectively. Concerning existence, uniqueness and regularity of a solution of (2.5)–(2.9), we refer to [6].

3. Time-discrete Cahn-Hilliard system

We integrate (2.5)–(2.9) in time by utilizing a semi-implicit Euler scheme. For this purpose, let $u^\tau_{\text{old}} \in H^1(\Omega)$ and $u^\tau \in H^1(\Omega)$ denote the time-discrete solution at t_{old} and $t = t_{\text{old}} + \tau$, respectively. Here, $\tau > 0$ denotes the (uniform) time-step size. Then u^τ with associated w^τ solves the problem: Find $u \in \mathcal{K}$ and $w \in H^1(\Omega)$ such that

$$(u,v) + \tau(\nabla w, \nabla v) \quad = \quad (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{3.1}$$

$$\gamma(\nabla u, \nabla v - \nabla u) - (w, v-u) \quad \ge \quad (u_{old}, v-u) \quad \forall v \in \mathcal{K}. \tag{3.2}$$

We mention that in [7] an unconditional gradient stability result for the discretization scheme (3.1)–(3.2) was established. In order to ease the notation, from now on we write u and u_{old} instead of u^τ and u^τ_{old}, respectively.

Following [21, 22], it is convenient to interpret (3.1)–(3.2) as the first order optimality system of an optimization problem. For the formulation of the latter we define the Sobolev space

$$V_0 = \left\{ v \in H^1(\Omega) : \ (v, 1) = 0 \right\},$$

and assume, without loss of generality, that $(u_0, 1) = 0$, $(u_{old}, 1) = 0$ and $|\Omega| = 1$ hold true. We further use $\|\cdot\|$ for the L^2-norm. For the minimization problem

$$(\mathcal{P}) \quad \min_{(u,w)\in\mathcal{K}\times V_0} J(u,w) := \frac{\gamma}{2}\|\nabla u\|^2 + \frac{\tau}{2}\|\nabla w\|^2 - (u_{old}, u) \quad \text{subject to} \quad (3.1)$$

we have the following result.

Lemma 3.1. *Let $\mathcal{F}$ be the feasible set of $(\mathcal{P})$. Then the following properties hold true:*

(i) *$\mathcal{F} \neq \emptyset$ and $\mathcal{F} \subset V_0 \times V_0$.*
(ii) *$\mathcal{F}$ is a closed convex set of $H^1(\Omega) \times H^1(\Omega)$.*
(iii) *J is strictly convex on $\mathcal{F}$.*
(iv) *For every sequence $(u_n, w_n)_{n\in\mathbb{N}}$ in $\mathcal{F}$ such that $\lim\limits_{n\to\infty} \|u_n\|_{H^1(\Omega)} = +\infty$ or $\lim\limits_{n\to\infty} \|w_n\|_{H^1(\Omega)} = +\infty$ we have $\lim_{n\to\infty} J(u_n, w_n) = +\infty$.*

Proof. (i) We have $\mathcal{F} \neq \emptyset$ since $(u_{old}, 0) \in \mathcal{F}$. In addition, for all $(u, w) \in \mathcal{F}$ we have $w \in V_0$. By taking $v = 1$ in (3.1), we obtain $(u, 1) = (u_{old}, 1) = 0$. Therefore, $\mathcal{F} \subset V_0 \times V_0$.

(ii) The convexity of $\mathcal{F}$ follows from the convexity of $\mathcal{K} \times H^1(\Omega)$ and the linearity of (3.1). For the closedness of $\mathcal{F}$ consider a sequence $(u_n, w_n)_{n\in\mathbb{N}} \subset \mathcal{F}$ such that $(u_n, w_n) \to (u, w)$ in $H^1(\Omega) \times H^1(\Omega)$. Then,

$$(u_n, v) + \tau(\nabla w_n, \nabla v) = (u_{old}, v) \quad \forall v \in H^1(\Omega) \tag{3.3}$$

which, upon passing to the limit, yields (3.1). The requirement $|u| \leq 1$ a.e. in Ω follows from the weak closedness of $\mathcal{K}$.

(iii) Let (u_1, w_1), $(u_2, w_2) \in \mathcal{F}$ and $\alpha \in]0, 1[$. Setting

$$r(\alpha) := \ \alpha J(u_1, w_1) + (1-\alpha)J(u_2, w_2) - J(\alpha(u_1, w_1) + (1-\alpha)(u_2, w_2)),$$

we have $r(\alpha) = \frac{1}{2}\alpha(1-\alpha)(\|\nabla(u_1 - u_2)\|^2 + \|\nabla(w_1 - w_2)\|^2) \geq 0$. Moreover, $r(\alpha) = 0$ yields

$$\|\nabla(u_1 - u_2)\| = \|\nabla(w_1 - w_2)\| = 0. \tag{3.4}$$

Since $\mathcal{F} \subset V_0 \times V_0$, we deduce from the Poincaré-Friedrichs inequality and (3.4) that $(u_1, w_1) = (u_1, w_2)$. Consequently, J is strictly convex on $\mathcal{F}$.

(iv) By Young's inequality we have

$$J(u, w) \geq \frac{\gamma}{2}\|\nabla u\|^2 + \frac{\tau}{2}\|\nabla w\|^2 - \frac{\beta}{2}\|u\|^2 - \frac{1}{2\beta}\|u_{old}\|^2$$

for all $(u,w) \in \mathcal{F}$ and for all $\beta > 0$. Again from $\mathcal{F} \subset V_0 \times V_0$ and the Poincaré-Friedrichs inequality we infer

$$J(u,w) \geq \frac{(\kappa - \beta C_p)}{2}\|\nabla u\|^2 + \frac{\tau}{2}\|\nabla w\|^2 - \frac{1}{2\beta}\| u_{old}\|^2 \qquad \forall \beta > 0.$$

Consequently, (iv) follows from choosing β such that $\gamma - \beta C_p > 0$. □

The relation between $(\mathcal{P})$ and (3.1)–(3.2) is established next.

Theorem 3.2. *The problem $(\mathcal{P})$ has a unique solution $(u^\star, w^\star)$. Moreover there exists a Lagrange multiplier $p^\star \in H^1(\Omega)$ such that $w^\star = p^\star - (p^\star, 1)$ and $(u^\star, p^\star)$ is a solution of (3.1)–(3.2). Conversely, if $(u^\star, p^\star)$ is a solution to (3.1)–(3.2), then $(u^\star, w^\star)$ with $w^\star = p^\star - (p^\star, 1)$ is the unique solution of $(\mathcal{P})$.*

Proof. The existence and uniqueness of the solution of $(\mathcal{P})$ are immediate consequences of the previous lemma. The existence of a Lagrange multiplier $p^\star$ follows from mathematical programming in Banach space; see, e.g., [33]. In order to keep the paper selfcontained we repeat the main result in the appendix and check here that the constraint qualification (8.2) is satisfied. For a given $f \in H^1(\Omega)^*$, in our context it consists in finding $(u,w) \in \mathcal{K} \times V_0$ and $\xi \geq 0$ such that

$$\tau(\nabla w, \nabla v) = \langle f, v\rangle - \xi(u - u^\star, v) =: g \quad \forall v \in H^1(\Omega). \tag{3.5}$$

Let $u \in \mathcal{K}$ such that $(u,1) \neq 0$ and $\xi = \langle f, 1\rangle/(u,1) \geq 0$. Its existence is guaranteed since $\mathcal{K}$ is symmetric with respect to the origin. Note that the right hand side $g \in H^1(\Omega)^*$ in (3.5) satisfies the compatibility condition $\langle g, 1\rangle = 0$. Hence, by the Lax-Milgram theorem there exists a unique w such that (3.5) is fullfilled. Now Theorem 8.1 yields the existence of an adjoint state (or Lagrange multiplier associated with (3.1)) $p^\star \in H^1(\Omega)$ such that

$$(u^\star, v) + \tau(\nabla w^\star, \nabla v) = (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{3.6}$$

$$\gamma\,(\nabla u^\star, \nabla(v - u^\star)) - (p^\star, v - u^\star) \geq (u_{old}, v - u^\star) \quad \forall v \in \mathcal{K}, \tag{3.7}$$

$$(\nabla p^\star, \nabla v) = (\nabla w^\star, \nabla v) \quad \forall v \in H^1(\Omega). \tag{3.8}$$

Consequently, $(u^\star, p^\star)$ is a solution of (3.1)–(3.2).

For the reverse implication it is clear that if $(u^\star, p^\star)$ is a solution of (3.1)–(3.2), then $(u^\star, w^\star, p^\star)$ with $w^\star = p^\star - (p^\star, 1)$ is a solution of the optimality system (3.6)–(3.8). Since $(\mathcal{P})$ is a convex problem, any stationary point of $(\mathcal{P})$, i.e. a solution of (3.6)–(3.8), is also a global solution of $(\mathcal{P})$. Thus, $(u^\star, w^\star)$ is the unique solution of $(\mathcal{P})$. □

4. Moreau-Yosida regularized problem

It is well-known that variational inequalities like (3.7) may be reformulated as complementarity systems by introducing Lagrange multipliers associated with the constraints in $\mathcal{K}$. Since $u \in H^1(\Omega)$, these multipliers are elements of $H^1(\Omega)^*$, thus not allowing a pointwise interpretation. This low regularity complicates the numerical treatment and might have an adverse effect on the convergence rate of an associated solution method. For this purpose we replace the above optimization problem by its Moreau-Yosida regularized version

$$(\mathcal{P}_c) \qquad \min_{(u,w)\in H^1(\Omega)\times V_0} J_c(u,w) \quad \text{subject to (3.1)}$$

with the objective

$$J_c(u,w) := J(u,w) + \frac{c}{2}\|\max(0,u-1)\|^2 + \frac{c}{2}\|\min(0,u+1)\|^2,$$

where $c > 0$ denotes the associated regularization (or, due to the structure of the additional terms, penalty) parameter. Note that the max- and min-expressions arise from regularizing the indicator function of $\mathcal{K}$.

We analyse $(\mathcal{P}_c)$ and start with a result similar to Theorem 3.2.

Theorem 4.1. *The problem $(\mathcal{P}_c)$ has a unique solution (u_c, w_c). Moreover, there exists a unique $p_c \in H^1(\Omega)$ such that*

$$p_c - (p_c, 1) = w_c, \tag{4.1}$$

$$\tau(\nabla p_c, \nabla v) + (u_c, v) - (u_{old}, v) = 0 \quad \forall v \in H^1(\Omega), \tag{4.2}$$

$$\gamma(\nabla u_c, \nabla v) + (\lambda_c(u_c), v) - (p_c, v) - (u_{old}, v) = 0 \quad \forall v \in H^1(\Omega), \tag{4.3}$$

where $\lambda_c(u_c) = \lambda_c^+(u_c) + \lambda_c^-(u_c)$ with

$$\lambda_c^+(u_c) := c\max(0, u_c - 1) \quad \text{and} \quad \lambda_c^+(u_c) := c\min(0, u_c + 1).$$

Conversely, if (u_c, p_c) is a solution of (4.2)–(4.3) then (u_c, w_c) with $w_c = p_c - (p_c, 1)$ is the unique solution of $(\mathcal{P}_c)$.

Proof. We start by noting that the functionals $u \to \|\max(0, u-1)\|^2$ and $u \to \|\min(0, u+1)\|^2$ are convex and Fréchet-differentiable on $H^1(\Omega)$ and that $\mathcal{F}_c$, the feasible set of $(\mathcal{P}_c)$, as well as J_c satisfy the analogue of Lemma 3.1 for $(\mathcal{P}_c)$. Hence, $(\mathcal{P}_c)$ is a convex problem whose cost function is radially unbounded and strictly convex. This yields existence and uniqueness of (u_c, w_c). Similarly, as in the proof of Theorem 3.2, mathematical programming theory in Banach space guarantees the existence of an adjoint state $p_c \in H^1(\Omega)$ satisfying the following first-order optimality system of $(\mathcal{P}_c)$:

$$(u_c, v) + \tau(\nabla w_c, \nabla v) = (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{4.4}$$

$$\gamma(\nabla u_c, \nabla v) + (\lambda_c(u_c), v) - (p_c, v) = (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{4.5}$$

$$(\nabla p_c, \nabla v) = (\nabla w_c, \nabla v) \quad \forall v \in H^1(\Omega). \tag{4.6}$$

Observe that (4.6) is equivalent to $w_c = p_c - \zeta$ for some $\zeta \in \mathbb{R}$. From $w_c \in V_0$ we deduce that $\zeta = (p_c, 1)$. Thus, (4.4)–(4.6) is equivalent to

$$(u_c, v) + \tau(\nabla p_c, \nabla v) = (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{4.7}$$

$$\gamma(\nabla u_c, \nabla v) - (p_c, v) + (\lambda_c(u_c), v) = (u_{old}, v) \quad \forall v \in H^1(\Omega), \tag{4.8}$$

$$w_c = p_c - (p_c, 1). \tag{4.9}$$

The uniqueness of p_c follows from the uniqueness of (u_c, w_c), the solution of $(\mathcal{P}_c)$, and (4.8). $\square$

The relation between $(\mathcal{P})$ and $(\mathcal{P}_c)$ is studied in the following proposition.

Proposition 4.2. *Let $\{(u_c, w_c)\}_{c>0}$ be a sequence of solutions of $(\mathcal{P}_c)$ as $c \to +\infty$. Then there exists a subsequence still denoted by $\{(u_c, w_c)\}_{c>0}$ such that*

$$(u_c, w_c) \to (u^\star, w^\star) \text{ in } H^1(\Omega) \tag{4.10}$$

as $c \to +\infty$, where $(u^\star, w^\star)$ is the unique solution of $(\mathcal{P})$. In particular, $u^\star$ is the order parameter corresponding to the solution of (3.1)–(3.2).

Proof. By the properties of the respective solutions, we have

$$J(u_c, w_c) \le J_c(u_c, w_c) \le J_c(u^\star, w^\star) = J(u^\star, w^\star). \tag{4.11}$$

Therefore, there exists a constant $\beta > 0$ independent of c such that

$$\frac{\gamma}{2}\|\nabla u_c\|^2 + \frac{\tau}{2}\|\nabla w_c\|^2 - (u_{old}, u_c) + \frac{c}{2}\|\max(0, u_c - 1)\|^2 + \frac{c}{2}\|\min(0, u_c + 1)\|^2 \le \beta.$$

Since $\mathcal{F}_c \subset V_0 \times V_0$, the Poincaré-Friedrichs inequality and Young's inequality yield

$$\{u_c\} \quad \text{bounded in} \quad H^1(\Omega), \tag{4.12}$$

$$\{w_c\} \quad \text{bounded in} \quad H^1(\Omega), \tag{4.13}$$

$$\{\sqrt{c}\max(0, u_c - 1)\} \quad \text{bounded in} \quad L^2(\Omega), \tag{4.14}$$

$$\{\sqrt{c}\min(0, u_c + 1)\} \quad \text{bounded in} \quad L^2(\Omega). \tag{4.15}$$

Consequently, there exist $(u, w) \in H^1(\Omega) \times H^1(\Omega)$ and a subsequence still denoted by $\{(u_c, w_c)\}_{c>0}$ such that

$$(u_c, w_c) \to (u, w) \text{ in } L^2(\Omega) \quad \text{and} \quad (u_c, w_c) \rightharpoonup (u, w) \text{ in } H^1(\Omega) \tag{4.16}$$

as $c \to +\infty$. Moreover, passing to the limit in the state equation of $(\mathcal{P}_c)$, we obtain

$$(u, v) + \tau(\nabla w, \nabla v) \;=\; (u_{old}, v) \quad \forall v \in H^1(\Omega). \tag{4.17}$$

On the other hand, from (4.16) and Lebesgue's dominated convergence theorem we infer

$$\max(0, u_c - 1) \;\to\; \max(0, u - 1) \text{ in } L^2(\Omega), \tag{4.18}$$

$$\min(0, u_c + 1) \;\to\; \min(0, u + 1) \text{ in } L^2(\Omega). \tag{4.19}$$

This together with (4.14)–(4.15) yields

$$-1 \le u \le 1 \quad \text{a.e. in } \Omega. \tag{4.20}$$

From (4.17) and (4.20) we deduce that $(u, w) \in \mathcal{F}$. Moreover, from (4.11) and the lower semi-continuity of semi-norms in $H^1(\Omega)$ we infer

$$J(u, w) \le \liminf_{c \to \infty} J(u_c, w_c) \le J(u^\star, w^\star). \tag{4.21}$$

The uniqueness of the solution of $(\mathcal{P})$ implies $(u, w) = (u^\star, w^\star)$.

Finally, we establish the strong convergence result in $H^1(\Omega)$. For this purpose note that (4.11) and (4.21) imply

$$\frac{c}{2}\|\max(u_c-1,0)\|^2+\frac{c}{2}\|\min(u_c+1,0)\|^2 \to 0 \quad \text{as } c\to+\infty.$$

Hence, we have

$$J(u^\star,w^\star)\le \liminf_{c\to\infty} J_c(u_c,w_c)\le \limsup_{c\to\infty} J_c(u_c,w_c)\le J(u^\star,w^\star)$$

and further

$$\lim_{c\to\infty}\|\nabla u_c\|=\|\nabla u^\star\| \quad \text{as well as} \quad \lim_{c\to\infty}\|\nabla w_c\|=\|\nabla w^\star\|.$$

Now, the weak and norm convergence yield the strong convergence result (4.10). ☐

Concerning the limit of the first order optimality system (4.1)–(4.3) we first establish an auxiliary result.

Lemma 4.3. *There exist constants $\beta_p>0$ and $\beta_\lambda>0$ independent of c, respectively, such that*

$$|(p_c,1)|\le\beta_p, \tag{4.22}$$

$$\|\lambda_c(u_c)\|\le\|\lambda_c^+(u_c)\|+\|\lambda_c^-(u_c)\|\le\beta_\lambda, \tag{4.23}$$

for all $c>0$.

Proof. We start by observing that

$$(p_c,u_c)=(w_c+(p_c,1)1,u_c)=(w_c,u_c) \tag{4.24}$$

since $((p_c,1)1,u_c)=(p_c,1)(u_c,1)=0$. Moreover, we have

$$(\min(u_c+1,0),u_c-1)\ge 0 \quad \text{and} \quad (\max(u_c-1,0),u_c+1)\ge 0 \tag{4.25}$$

as $\min(u_c(x)+1,0)=u_c(x)+1$ implies $u_c(x)+1\le 0$ and thus $u_c(x)-1\le -2$ and analogously for the second estimate above.

Considering now (4.3) and the definition of $\lambda_c(u_c)$, then choosing $v=u_c-1\in H^1(\Omega)$ yields

$$\begin{aligned}0&=\gamma\|\nabla u_c\|^2+c\|\max(u_c-1,0)\|^2+c(\min(u_c+1,0),u_c-1)-(p_c,u_c)\\&\quad+(p_c,1)-(u_{old},u_c)\\&\ge(p_c,1)-(w_c+u_{old},u_c),\end{aligned}$$

where we used (4.24), (4.25) and $(u_{old},1)=0$. Due to the boundedness of $\{\|w_c\|_{H^1}\}$ and $\{\|u_c\|_{H^1}\}$ there exists $\beta_p>0$ such that

$$(p_c,1)\le\|u_c\|(\|w_c\|+\|u_{old}\|)\le\beta_p \quad \text{for all } c>0. \tag{4.26}$$

For the reverse estimate consider again (4.3) with $v=u_c+1\in H^1(\Omega)$. Then, we have

$$\begin{aligned}0&=\gamma\|\nabla u_c\|^2+c\|\min(u_c+1,0)\|^2+c(\max(u_c-1,0),u_c+1)-(p_c,u_c)\\&\quad-(p_c,1)-(u_{old},u_c)\\&\ge-(p_c,1)-(w_c+u_{old},u_c),\end{aligned}$$

and consequently

$$(p_c, 1) \geq -\|u_c\|(\|w_c\| + \|u_{old}\|) \geq -\beta_p \quad \text{for all } c > 0. \tag{4.27}$$

Combining (4.26) and (4.27) yields (4.22).

For showing (4.23) we first use $v = \lambda_c^+(u_c) = c\max(0, u_c - 1) \in H^1(\Omega)$ and then $v = \lambda_c^-(u_c) = c\min(0, u_c + 1) \in H^1(\Omega)$ in (4.3), respectively. As a consequence, we get

$$\gamma c\|\nabla \max(u_c - 1, 0)\|^2 + \|\lambda_c^+(u_c)\|^2 - (p_c, \lambda_c^+(u_c)) - (u_{old}, \lambda_c^+(u_c)) = 0$$

and

$$\gamma c\|\nabla \min(u_c + 1, 0)\|^2 + \|\lambda_c^-(u_c)\|^2 - (p_c, \lambda_c^-(u_c)) - (u_{old}, \lambda_c^-(u_c)) = 0,$$

yielding

$$\|\lambda_c^+(u_c)\|^2 \leq \|p_c\|\|\lambda_c^+(u_c)\| + \|u_{old}\|\|\lambda_c^+(u_c))\|$$

and

$$\|\lambda_c^-(u_c)\|^2 \leq \|p_c\|\|\lambda_c^-(u_c)\| + \|u_{old}\|\|\lambda_c^-(u_c))\|,$$

which prove (4.23). □

This allows us to study the limit of (4.2)–(4.3) as $c \to \infty$.

Theorem 4.4. *For $c \to \infty$ there exists $p^\star \in H^1(\Omega)$ and a subsequence of $\{p_c\}$ which converges to $p^\star$ weakly in $H^1(\Omega)$. Moreover, together with $(u^\star, w^\star)$ of Proposition 4.2 $p^\star$ satisfies the first order optimality system* (3.6)–(3.8).

Proof. The weak convergence of $\{p_c\}$ in $H^1(\Omega)$ to $p^\star$ along a subsequence follows from the uniform boundedness of $\{w_c\}$ in $H^1(\Omega)$, $p_c = w_c + (p_c, 1)$ and the uniform boundedness of $\{|(p_c, 1)|\}$ according to Lemma 4.3.

Concerning the first order system (3.6)–(3.8) we note that (3.8) follows immediately from (4.1) and the boundedness properties of $\{w_c\}$ respectively $\{p_c\}$. Equation (3.6) was already established in the proof of Proposition 4.2. It remains to study (3.7). For this purpose observe that for arbitrarily fixed $v \in \mathcal{K}$ the following holds:

$$\begin{aligned}(\lambda_c(u_c), v - u_c) &= c(\max(u_c - 1, 0), v - u_c) + c(\min(u_c + 1, 0), v - u_c)\\ &= c(\max(u_c - 1, 0), v - 1) + c(\max(u_c - 1, 0), 1 - u_c)\\ &\qquad + c(\min(u_c + 1, 0), v + 1), + c(\min(u_c + 1, 0), -1 - u_c)\\ &\leq 0,\end{aligned}$$

where we used $-1 \leq v \leq 1$ a.e. in Ω. Hence, we have

$$\lim_{c\to\infty} (\lambda_c(u_c), v - u_c) \leq 0.$$

Next, recall that due to Proposition 4.2 we have the strong convergence of $\{u_c\}$ in $H^1(\Omega)$ and by Lemma 4.3 the uniform boundedness of $\{\lambda_c(u_c)\}$ in $L^2(\Omega)$, respectively. Therefore, from the last estimate above together with passing to the limit in (4.3) with $v \in H^1(\Omega)$ replaced by $v - u_c$ with $v \in \mathcal{K}$ we obtain

$$\gamma(\nabla u^\star, \nabla(v - u^\star)) - (p^\star, v - u^\star) \geq (u_{old}, v - u^\star) \quad \forall v \in \mathcal{K},$$

which establishes (3.7). $\square$

Remark 4.5. Solving the optimality system (4.2)–(4.3) for a sequence $\{c\}$, with $c \geq \underline{c} > 0$ and $c \to +\infty$, constitutes an iterative way for solving the time-discrete Cahn-Hilliard system (3.1)–(3.2).

5. Semi-Smooth Newton method for the regularized problems

The previous Remark 4.5 motivates our function space algorithm for solving the time-discrete Cahn-Hilliard problem. In fact, we specify a sequence $c \to \infty$ and solve the optimality system (4.2)–(4.3), here compactly written as

$$F_c(u_c, w_c) = (F_c^{(1)}(u_c, w_c), F_c^{(2)}(u_c, w_c)) = 0, \tag{5.1}$$

for every c by a semi-smooth Newton algorithm. In (5.1) the components are defined by

$$\left\langle F_c^{(1)}(u, w), v \right\rangle = \tau(\nabla w, \nabla v) + (u, v) - (u_{old}, v), \tag{5.2}$$

$$\left\langle F_c^{(2)}(u, w), v \right\rangle = \gamma(\nabla u, \nabla v) + (\lambda_c(u), v) - (w, v) - (u_{old}, v) \tag{5.3}$$

for all u, w and v in $H^1(\Omega)$. Due to the presence of the max- and min-operators in the definition of λ_c, F_c is not Fréchet-differentiable. However, it satisfies the weaker notion of Newton-differentiability [23], which we recall next.

Definition 5.1. Let X and Z be Banach spaces, $D \subset X$ an open subset. A mapping $F : D \subset X \to Z$ is called Newton-differentable in $U \subset D$ if there exists a family of mappings $G : U \to Z$ such that

$$\lim_{d \to 0} \frac{1}{\|d\|_X} \|F(x + d) - F(x) - G(x + d)d\|_Z = 0 \qquad \forall x \in U.$$

The operator G is called a Newton-derivative of F on U.

In finite dimensions, Newton-differentiability resembles the concept of semi-smoothness [32, 29]. For Newton-differentiable mappings the following convergence result for the (semi-smooth) Newton iteration

$$x^{k+1} = x^k - G(x^k)^{-1} F(x^k) \quad \text{for } k = 0, 1, \ldots \tag{5.4}$$

holds true. For its proof we refer to [23].

Theorem 5.2. *Let $x^\star$ be a solution of $F(x) = 0$, and suppose that $F : D \subset X \to Z$ is Newton-differentiable in a neighborhood U of $x^\star$ with $\left\{\|G(x)^{-1}\|_{\mathcal{L}(Z,X)} : \quad x \in U\right\}$ bounded. Then the sequence $\{x^k\}_{k \in \mathbb{N}}$ generated by (5.4) converges superlinearly to $x^\star$ provided that $\|x^0 - x^\star\|_X$ is sufficiently small.*

Our goal is to apply Theorem 5.2 to (4.2)–(4.3). For this purpose we establish the following auxiliary results.

Lemma 5.3. *The mapping $F_c : H^1(\Omega) \times H^1(\Omega) \to H^1(\Omega)^* \times H^1(\Omega)^*$ is Newton-differentiable. Furthermore, the operator $G_c(u,w)$ given by*

$$\langle G_c(u,w)(\delta u, \delta w), (\phi, \psi)\rangle = \begin{pmatrix} \tau(\nabla \delta w, \nabla \phi) + (\delta u, \phi) \\ \gamma(\nabla \delta u,\ \nabla \psi) + c(\chi_{\mathcal{A}(u)}\delta u, \psi) - (\delta w, \psi) \end{pmatrix}$$

serves as a Newton-derivative for F_c, where $\chi_{\mathcal{A}(u)}$ is the characteristic function of the set

$$\mathcal{A}(u) := \{x \in \Omega :\ u(x) \geq 1\} \cup \{x \in \Omega :\ u(x) \leq -1\}.$$

Proof. According to [23], the mappings $\max(0,.) : L^s(\Omega) \to L^r(\Omega)$ and $\min(0,.) : L^s(\Omega) \to L^r(\Omega)$ with $1 \leq r < s \leq \infty$ are Newton-differentiable on $L^s(\Omega)$ with Newton-derivatives

$$G_{\max}(y)(x) = \begin{cases} 1 & \text{if} \quad y(x) \geq 0, \\ 0 & \text{if} \quad y(x) < 0 \end{cases} \tag{5.5}$$

and

$$G_{\min}(y)(x) = \begin{cases} 1 & \text{if} \quad y(x) \leq 0, \\ 0 & \text{if} \quad y(x) > 0. \end{cases} \tag{5.6}$$

Moreover, $H^1(\Omega)$ is continuousely embedded in $L^s(\Omega)$ for some $s = s(n) > 2$ by Sobolev embedding. Furthermore, $L^r(\Omega)$ with $2 \leq r < s$ is continuously embedded in $H^1(\Omega)^*$. Therefore, the max- and min-mappings considered from $H^1(\Omega)$ to $H^1(\Omega)^*$ are Newton-differentiable with $G_{\max}$ and $G_{\min}$, respectively, as associated Newton-derivatives.

Further it is clear that Fréchet-differentiability implies Newton differentiability. Hence, F_c is Newton-differentiable. By using Definition 1 directly, one readily checks that G_c serves as a Newton-derivative for F_c. □

Lemma 5.4. *For given u in $H^1(\Omega)$ and (y_1, y_2) in $H^1(\Omega)^* \times H^1(\Omega)^*$, the optimization problem*

$(\mathcal{P}_{G_c})$

$$\begin{array}{ll} \displaystyle\min_{(\delta u, \delta p) \in H^1(\Omega) \times V_0} & \dfrac{\gamma}{2}\|\nabla \delta u\|^2 + \dfrac{\tau}{2}\|\nabla \delta p\|^2 + c(\chi_{\mathcal{A}(u)}\delta u, \delta u) - (y_2, \delta u) \\ \text{subject to} & \tau(\nabla \delta p, \nabla \phi) + (\delta u, \phi) = (y_1, \phi) \quad \forall \phi \in H^1(\Omega) \end{array}$$

admits a unique solution $(\delta u, \delta p)$. Moreover, there exists a unique $\delta w \in H^1(\Omega)$ such that

$$\tau(\nabla \delta w, \nabla \phi) + (\delta u, \phi) = (y_1, \phi), \tag{5.7}$$

$$\gamma(\nabla \delta u,\ \nabla \psi) + c(\chi_{\mathcal{A}(u)}\delta u, \psi) - (\delta w, \psi) = (y_2, \psi) \tag{5.8}$$

for all ψ and ϕ in $H^1(\Omega)$. Conversely, if $(\delta u, \delta w)$ is a solution of (5.7)–(5.8) then $(\delta u, \delta p)$ with $\delta p = \delta w - (\delta w, 1)$ is the unique solution of $(\mathcal{P}_{G_c})$.

Proof. One proceeds as in the proofs of Theorems 3.2 and 4.1. □

Proposition 5.5. *The mapping $F_c : H^1(\Omega) \times H^1(\Omega) \to H^1(\Omega)^* \times H^1(\Omega)^*$ is Newton-differentiable. A specific Newton-derivative G_c is given by*

$$\langle G_c(u,w)(\delta u, \delta w), (\phi, \psi)\rangle = \begin{pmatrix} \tau(\nabla \delta w, \nabla \phi) + (\delta u, \phi) \\ \gamma(\nabla \delta u,\ \nabla \psi) + c(\chi_{AS(u)}\delta u, \psi) - (\delta w, \psi) \end{pmatrix}$$

with δu, δw, ϕ, $\psi \in H^1(\Omega)$. Moreover, the semi-smooth Newton iteration (5.4) *(with F and G replaced by F_c and G_c) converges superlinearly to (u_c, w_c), the solution of* (4.2)–(4.3)*, provided that $\|(u^0, w^0)-(u_c, w_c)\|_{H^1(\Omega)\times H^1(\Omega)}$ is sufficiently small.*

Proof. The Newton-differentiability of F_c as well as a specific Newton-derivative are given by Lemma 5.3.

From Lemma 5.4 we deduce that, for all $(u, w) \in H^1(\Omega)\times H^1(\Omega)$, $G_c(u, w)$ is invertible, i.e., for given $(y_1, y_2) \in H^1(\Omega)^* \times H^1(\Omega)^*$ there exists a unique pair $(\delta u, \delta w) \in H^1(\Omega) \times H^1(\Omega)$ such that (5.7)–(5.8) is satisfied. Taking $(\phi, \psi) = (\delta u, \delta w)$ in (5.7)–(5.8) and adding the two equations we obtain

$$\gamma\|\nabla\delta u\|^2 + \tau\|\nabla\delta w\|^2 + c(\chi_{\mathcal{A}(u)}\delta u, \delta u) = (y_2, \delta u) + (y_1, \delta w).$$

From this we infer

$$\gamma\|\nabla\delta u\|^2 + \tau\|\nabla\delta w\|^2 \leq C(\|y_1\|^2_{H^1(\Omega)^*} + \|y_2\|^2_{H^1(\Omega)^*}), \tag{5.9}$$

where the (generic) constant $C > 0$ possibly depends on γ, τ or c, but not on δu or δw. Moreover, from (5.7)–(5.8) we get

$$(\delta u, 1) = (y_1, 1) \text{ and } (\delta w, 1) = c(\chi_{\mathcal{A}(u)}\delta u, 1) - (y_2, 1). \tag{5.10}$$

From (5.9), (5.10) and the Poincaré-Friedrichs inequality it follows that

$$\|(\delta u, \delta w)\|_{H^1(\Omega)\times H^1(\Omega)} \leq C(\|y_1\|_{H^1(\Omega)^*} + \|y_2\|_{H^1(\Omega)^*}). \tag{5.11}$$

For $\max(\|y_1\|_{H^1(\Omega)^*}, \|y_2\|_{H^1(\Omega)^*}) \leq \beta$ for some constant $\beta > 0$, we consequently have

$$\|G_c^{-1}(u, w)\|_{\mathcal{L}(H^1(\Omega)^2,(H^1(\Omega)^*)^2)} \leq \hat{C} \qquad \forall(u, w) \in H^1(\Omega) \times H^1(\Omega)$$

with some constant $\hat{C} > 0$ possibly depending on γ, τ, c or β, but independent of u, w. Thus, F_c with associated Newton-derivative G_c fulfills the conditions of Theorem 5.2, which completes the proof. □

6. Finite element approximation

For computational purposes we next discretize (4.2)–(4.3) by finite elements. Further, in order to enhance the computational performance of the resulting discrete semi-smooth Newton solver, in the following section we intertwine our solver with an adaptive finite element method based on residual-type a posteriori error estimators.

Consider a shape-regular simplicial triangulation $\mathcal{T}_h$ of Ω. For convenience we assume that Ω is polyhedral such that the boundary $\partial\Omega$ is exactly represented by the boundaries of triangles $T \in \mathcal{T}_h$; otherwise we assume the elements lying on the boundary to be curved. We refer to $\mathcal{N}_h = \cup_{i=1}^N\{x_i\}$ and $\mathcal{E}_h$ as the set of nodes and interior edges of $\mathcal{T}_h$, respectively. For each element T in $\mathcal{T}_h$, we denote by h_T and $|T|$ the diameter and area of T, respectively. Further, for an edge $E \in \mathcal{E}_h$, h_E stands for the length of E. We associate with $\mathcal{T}_h$ the piecewise linear finite element space

$$\mathcal{V}_h = \{v \in C_0(\overline{\Omega}) : v|_T \in P_1(T), \forall T \in \mathcal{T}_h\},$$

where $P_1(T)$ is the space of first-order polynomials on T. The standard nodal basis of $\mathcal{V}_h$, denoted by $\{(\phi_i)\}_{i=1}^N$, satisfies $\phi_i(x_j) = \delta_{ij}$ for all x_j in $\mathcal{N}_h$ and $i, j \in 1, \ldots, N$. Here, δ_{ij} represents the Kronecker symbol.

The discretized version of the penalized problem (4.2)–(4.3) consists in finding (u_c^h, w_c^h) in $\mathcal{V}_h \times \mathcal{V}_h$ such that

$$\left\langle F_{c,h}^{(1)}(u_c^h, w_c^h), v^h \right\rangle = 0 \qquad \forall v^h \in \mathcal{V}_h, \tag{6.1}$$

$$\left\langle F_{c,h}^{(2)}(u_c^h, w_c^h), \psi^h \right\rangle = 0 \qquad \forall \psi^h \in \mathcal{V}_h. \tag{6.2}$$

For all (v, ψ) in $H^1(\Omega) \cap C_0(\overline{\Omega}) \times H^1(\Omega) \cap C_0(\overline{\Omega})$, we have

$$\left\langle F_{c,h}^{(1)}(u_c^h, w_c^h), v \right\rangle = \tau(\nabla w_c^h, \nabla v) + (u_c^h, v)^h - (u_{old}, v)^h, \tag{6.3}$$

and

$$\left\langle F_{c,h}^{(2)}(u_c^h, w_c^h), \psi \right\rangle = \gamma(\nabla u_c^h, \nabla\psi) + (\lambda_c(u_c^h), \psi)^h - (w_c^h, \psi)^h - (u_{old}, \psi)^h. \tag{6.4}$$

Here and in what follows, u_{old} is assumed to be a finite element function (i.e. $u_{old} \in \mathcal{V}_h$). The semi-inner product $(.\,,\,.)^h$ on $C_0(\overline{\Omega})$ is defined by

$$(f, g)^h := \int_\Omega \pi^h(f(x)g(x))dx = \sum_{i=1}^N (1, \phi_i) f(x_i) g(x_i) \quad \forall f,\, g \in C_0(\overline{\Omega}), \tag{6.5}$$

where $\pi^h : C_0(\overline{\Omega}) \to \mathcal{V}_h$ is the Lagrange interpolation operator. The induced semi-norm $|\,.\,|_h = \sqrt{(.\,,\,.)^h}$ satisfies

$$|g|_h \le \|g\| \le C|g|_h \qquad \forall g \in C_0(\overline{\Omega}), \tag{6.6}$$

where $C > 0$ is a constant depending only on Ω; see [5], for instance.

Within our finite element framework, for a given $(u^h, w^h) \in \mathcal{V}_h \times \mathcal{V}_h$, every step of the semi-smooth Newton method for solving (6.1)–(6.2) requires to compute $(\delta u^h, \delta w^h) \in \mathcal{V}_h \times \mathcal{V}_h$ satisfying

$$\tau(\nabla \delta w^h, \nabla v^h) + (\delta u^h, v^h)^h = -F_{c,h}^{(1)}(u^h, w^h) \quad \forall v^h \in \mathcal{V}_h, \tag{6.7}$$

$$\gamma(\nabla \delta u^h, \nabla \psi^h) + c(\chi_{\mathcal{A}(u^h)}^h \delta u^h, \psi^h)^h - (\delta w^h, \psi^h)^h = -F_{c,h}^{(2)}(u^h, w^h) \quad \forall \psi^h \in \mathcal{V}_h, \tag{6.8}$$

where $\chi_{\mathcal{A}(u^h)}^h := \sum_{i=1}^N \chi_{\mathcal{A}(u^h)}^h(x_i)\phi_i$ with $\chi_{\mathcal{A}(u^h)}^h(x_i) = 0$ if $-1 \le u^h(x_i) \le 1$ and $\chi_{\mathcal{A}(u^h)}^h(x_i) = 1$ otherwise.

In matrix form, the linear system (6.7)–(6.8) reads

$$\begin{pmatrix} A & -M \\ M & C \end{pmatrix} \begin{pmatrix} \delta U \\ \delta W \end{pmatrix} = \begin{pmatrix} B^{(2)} \\ B^{(1)} \end{pmatrix}, \tag{6.9}$$

where δU and δW are in $\mathbb{R}^N$, respectively, and

$$B_i^{(1)} = F_{c,h}^{(1)}(u^h, \phi_i), \quad B_i^{(2)} = F_{c,h}^{(2)}(u^h, \phi_i) \quad \forall i \in 1, \ldots, N, \tag{6.10}$$

$$C_{ij} = \tau(\nabla\phi_i, \nabla\phi_j), \quad M_{ij} = (\phi_i, \phi_j)^h \qquad \forall i, j \in 1, \ldots, N. \tag{6.11}$$

Further, the stiffness matrix A is given by

$$A = \gamma C + cM\, D(u^h)$$

with $D(u^h)$ is the diagonal matrix formed by $(\chi^h_{\mathcal{A}(u^h)}(x_i))_{i=1}^N$.
Note that C and A are symmetric and positive semi-definite matrices and M is a diagonal positive definite matrix. One readily finds that (6.9) is equivalent to

$$(M + CM^{-1}A)\delta U = B^{(1)} + CM^{-1}B^{(2)} \tag{6.12}$$

$$\delta W = M^{-1}(A\delta U - B^{(2)}). \tag{6.13}$$

Therefore, for solving (6.9) we propose the following Schur-complement based scheme:

$$\delta U = (M + CM^{-1}A)^{-1}(B^{(1)} + CM^{-1}B^{(2)}) \tag{6.14}$$

$$\delta W = M^{-1}(A\delta U - B^{(2)}). \tag{6.15}$$

Its justification is the subject of the following result.

Proposition 6.1. *The scheme* (6.14)–(6.15) *for solving* (6.9) *is well-defined.*

Proof. For the proof we use the fact that the product RS of real symmetric $N \times N$-matrices R and S with all of their eigenvalues in $[r_1, r_2]$ and $[s_1, s_2]$, with $0 \le r_1 \le r_2$ and $0 \le s_1 \le s_2$, respectively, has all of its eigenvalues in $[r_1 s_1, r_2 s_2]$.

Applying this result to $R := M^{-1}CM^{-1}$ and $S := A$ we deduce that $M^{-1}CM^{-1}A$ is positive semi-definite. Moreover, we have

$$(M + CM^{-1}A) = M(I + M^{-1}CM^{-1}A),$$

where I is the $N \times N$-identity matrix. Hence, $(M + CM^{-1}A)$ is positive definite and the system (6.14)–(6.15) is well-defined. □

As for the continuous problem (4.2)–(4.3), the solution of the finite element problem (6.1)–(6.2) is bounded in $H^1(\Omega)^2$ independently of the penalty parameter c.

Proposition 6.2. *Let* $\{(u_c^h, w_c^h)\}_{c>0}$ *be a sequence of solutions of* (6.1)–(6.2) *for* $c \to \infty$. *Then there exists a constant* C *independent of* c *such that*

$$\|u_c^h\|_{H^1(\Omega)} \le C, \tag{6.16}$$

$$\|w_c^h\|_{H^1(\Omega)} \le C, \tag{6.17}$$

$$\|\pi^h(\lambda_c(u_c^h)\|_{L^2(\Omega)} \le C. \tag{6.18}$$

Proof. We introduce the following discrete optimal control problem:
$(\mathcal{P}_c^h)$

$$\begin{aligned} &\min_{(u^h,p^h)\in\mathcal{V}_h\times\mathcal{V}_h\cap V_0} && J_h(u^h,p^h)+\frac{c}{2}|\max(0,u^h-1)|_h^2+\frac{c}{2}|\min(0,u^h+1)|_h^2 \\ &\text{subject to} && \tau(\nabla p^h,\nabla\phi^h)+(u^h-u_{old},\phi^h)^h=0 \quad \forall\phi^h\in\mathcal{V}_h, \end{aligned}$$

where

$$J_h(u^h,p^h):=\frac{\gamma}{2}\|\nabla u^h\|^2+\frac{\tau}{2}\|\nabla p^h\|^2-(u_{old},u^h)^h.$$

The mappings $u^h\to|\max(0,u^h-1)|_h^2$ and $u^h\to|\min(0,u^h+1)|_h^2$ for $u^h\in\mathcal{V}_h$ are continuously differentiable with

$$\begin{aligned} \frac{\partial}{\partial u^h}|\max(0,u^h-1)|_h^2 &= 2\,(\max(0,u^h-1),\,\cdot)^h, \\ \frac{\partial}{\partial u^h}|\min(0,u^h+1)|_h^2 &= 2\,(\min(0,u^h+1),\,\cdot)^h. \end{aligned}$$

Moreover we have

$$\begin{aligned} (v^h,1)^h &= (v^h,1) \qquad \forall v^h\in\mathcal{V}_h, \\ (\max(0,u^h-1),u^h-1)^h &= |\max(0,u^h-1)|_h^2, \\ (\min(0,u^h+1),u^h+1)^h &= |\min(0,u^h+1)|_h^2. \end{aligned}$$

Hence, by analogous reasoning as for the proofs of Proposition 4.2 and Lemma 4.3, it follows that $(u_c^h,w_c^h-(w_c^h,1))$ solves $(\mathcal{P}_c^h)$ with (6.16)–(6.17) holding true. Now to show (6.18) we introduce the function $v_c^h:=\sum_{i=1}^N v_c^h(x_i)\phi_i\in\mathcal{V}_h$ such that

$$v_c^h(x_i)=\begin{cases} \;\;1 & \text{if} \quad\;\; 1< u_c^h(x_i), \\ \;\;0 & \text{if} \quad -1\le u_c^h(x_i)\le 1, \\ -1 & \text{if} \quad -1> u_c^h(x_i), \end{cases}$$

which satisfies

$$\|v_c^h\|_{H^{1,\infty}(\Omega)}\le 1. \tag{6.19}$$

Moreover, we find

$$\begin{aligned} (\lambda_c(u_c^h)^+,v_c^h)^h &= c\int_\Omega \pi_h(\max(0,u_c^h(x)-1)v_c^h(x))dx, \\ &= c\int_\Omega \sum_{i=1}^N \max(0,u_c^h(x_i)-1)v_c^h(x_i)\phi_i(x)dx, \\ &= c\int_\Omega \sum_{i=1}^N \max(0,u_c^h(x_i)-1)\phi_i(x)dx, \\ &= \int_\Omega \pi_h(\lambda_c^+(u_c^h))dx, \\ &= \int_\Omega |\pi_h(\lambda_c^+(u_c^h))|dx, \end{aligned}$$

and similarly

$$(\lambda_c(u_c^h)^-, v_c^h)^h = \int_\Omega |\pi_h(\lambda_c^-(u_c^h))| dx. \tag{6.20}$$

Hence, we have

$$\begin{aligned}(\lambda_c(u_c^h),\, v_c^h)^h &= \|\pi_h(\lambda_c^+(u_c^h))\|_{L^1(\Omega)} + \|\pi_h(\lambda_c^-(u_c^h))\|_{L^1(\Omega)},\\ &\geq \|\pi_h(\lambda_c(u_c^h))\|_{L^1(\Omega)},\\ &\geq \beta\|\pi_h(\lambda_c(u_c^h))\|_{L^2(\Omega)}, \end{aligned}\tag{6.21}$$

with a generic constant $\beta > 0$ independent of c. Above the last inequality is obtained by the equivalence of norms in the finite-dimensional space $\mathcal{V}_h$. Multiplying (6.1) by v_c^h and using (6.6), (6.19), (6.21) and the fact that $(\cdot\,,\,\cdot)^h$ induces a semi-norm, we obtain

$$\|\pi_h(\lambda_c(u_c^h))\|_{L^2(\Omega)} \leq \beta(\|\nabla u_c^h\| + \|w_c^h\| + \|u_{old}\|), \tag{6.22}$$

from which, together with (6.16)–(6.17), one infers (6.18). □

7. A posteriori error estimation

In order to efficiently connect our Moreau-Yosida regularization based semismooth Newton solver to an adaptive finite element discretization, we next derive residual-type a posteriori error estimates for the finite element approximation of the regularized problem. We mention here that, based on the approach by [11], an a posteriori error analysis for a finite element discretization of the limit problem (3.1)–(3.2) was performed in [4].

For the ease of notation and as we are only referring to the Moreau-Yosida regularized problem, its solution and dual variables, in what follows we drop the parameter c from the notation of the solutions of the time-discrete problem and its finite element approximation. Thus, $(u, w) \in H^1(\Omega) \times H^1(\Omega)$ and $(u^h, w^h) \in \mathcal{V}_h \times \mathcal{V}_h$ refer to the solutions of (4.2)–(4.3) and (6.1)–(6.2), respectively. For $D \subset \Omega$ and $m \in \{0, 1\}$ we denote by $(\cdot,\cdot)_{m,D}$, $\|\cdot\|_{m,D}$ and $|\cdot|_{m,D}$ the standard inner product and the associated norm and semi-norm in $H^m(D)$, respectively.

We define the errors

$$e_u := u^h - u, \tag{7.1}$$

$$e_w := w^h - w, \tag{7.2}$$

$$e_{\lambda_c^h} := \pi_h(\lambda_c(u^h)) - \lambda_c(u^h), \tag{7.3}$$

$$e_{\lambda_c^+} := \lambda_c^+(u^h) - \lambda_c^+(u) := c(\max(0, u^h - 1) - \max(0, u - 1)), \tag{7.4}$$

$$e_{\lambda_c^-} := \lambda_c^-(u^h) - \lambda_c^-(u) := c(\min(0, u^h + 1) - \min(0, u + 1)), \tag{7.5}$$

the residuals

$$r^{(1)} := u - u_{old}, \tag{7.6}$$

$$r^{(2)} := \lambda_c(u) - w - u_{old}, \tag{7.7}$$

$$r_h^{(1)} := u^h - u_{old}, \tag{7.8}$$

$$r_h^{(2)} := \pi_h(\lambda_c(u^h)) - w^h - u_{old}, \tag{7.9}$$

the element residuals

$$\eta_T^{(1)} = h_T \|r_h^{(1)}\|_{0,T} \qquad \text{for all } T \in \mathcal{T}_h, \tag{7.10}$$

$$\eta_T^{(2)} = h_T \|r_h^{(2)}\|_{0,T} \qquad \text{for all } T \in \mathcal{T}_h, \tag{7.11}$$

$$\eta_T^{(3)} = \|e_{\lambda_c^h}\|_{0,T} \qquad \text{for all } T \in \mathcal{T}_h \tag{7.12}$$

and the so-called jump residuals

$$\eta_E^{(1)} = h_E^{1/2} \|[\nabla w^h]_E \cdot \boldsymbol{\nu}_E\|_{0,E} \qquad \text{for all } E \in \mathcal{E}_h, \tag{7.13}$$

$$\eta_E^{(2)} = h_E^{1/2} \|[\nabla u^h]_E \cdot \boldsymbol{\nu}_E\|_{0,E} \qquad \text{for all } E \in \mathcal{E}_h, \tag{7.14}$$

where, for all $E \in \mathcal{E}_h$, E is a common edge of T^+ and T^- with unit outward normals $\boldsymbol{\nu}_E^+$ and $\boldsymbol{\nu}_E^-$, respectively, and $\boldsymbol{\nu}_E = \boldsymbol{\nu}_E^-$. Further, to each function $f \in L^2(\Omega)$ we assign a piecewise constant function $\overline{f}$ defined by

$$\overline{f}_{|T} = \frac{1}{|T|}(f, 1)_{0,T} \qquad \text{for } T \in \mathcal{T}_h.$$

The local as well as the "regional" data oscillations are given by

$$\text{osc}_h(f, T) = \|h_T(f - \overline{f})\|_{0,T} \quad \text{for } T \in \mathcal{T}_h, \tag{7.15}$$

$$\text{osc}_h(f, D) = \left(\sum_{T \in D} \text{osc}_h(f, T)^2 \right)^{1/2} \qquad \text{for } D \subset \mathcal{T}_h. \tag{7.16}$$

By $\Pi_h : H^1(\Omega) \to \mathcal{V}_h$ we denote Clement's interpolation operator [12], which satisfies for each $T \in \mathcal{T}_h$ and $E \in \mathcal{E}_h$ that

$$\|v - \Pi_h v\|_{0,T} \le C h_T |v|_{1,\omega_T} \qquad \text{for all } v \in H^1(\Omega), \tag{7.17}$$

$$\|v - \Pi_h v\|_{0,E} \le C h_E^{1/2} |v|_{1,\omega_E} \quad \text{for all } v \in H^1(\Omega), \tag{7.18}$$

$$\|\Pi_h v\|_{0,T} \le C \|v\|_{0,T} \quad \text{for all } v \in H^1(\Omega), \tag{7.19}$$

$$|\Pi_h v|_{1,T} \le C |v|_{1,T} \quad \text{for all } v \in H^1(\Omega). \tag{7.20}$$

Here and below C denotes a generic positive constant depending only on the domain Ω and the smallest angle of the mesh $\mathcal{T}_h$. It may take different values at different occasions. Moreover, ω_T and ω_E are given by

$$\omega_T := \left\{ T' \in \mathcal{T}_h : \overline{T} \cap \overline{T'} \neq \emptyset \right\}, \tag{7.21}$$

$$\omega_E := \left\{ T \in \mathcal{T}_h : E \subset \overline{T} \right\}. \tag{7.22}$$

7.1. **Reliability of the estimator—a posteriori upper bound.** In what follows, we assume that Ω is convex or has a smooth boundary (of class $\mathcal{C}^2$). According to regularity results for the Neumann problem (see for instance [2, 28]) and in view of $w + u_{old} - \lambda(u) \in L^2(\Omega)$ and $u - u_{old} \in L^2(\Omega)$, the solution (u, w) belongs to $H^2(\Omega)^2$. Consequently, by the embedding of $H^2(\Omega)$ in $C_0(\overline{\Omega})$ for $n = 1, 2, 3$, the Lagrange interpolations of u and w are well defined. For all v in $H^1(\Omega)$, we have

$$\left\langle F_c^{(1)}(u,w), v \right\rangle = \left\langle F_c^{(2)}(u,w), v \right\rangle = 0. \tag{7.23}$$

This yields

$$\left\langle F_{c,h}^{(1)}(u^h,w^h), e_w \right\rangle = \left\langle F_{c,h}^{(1)}(u^h,w^h) - F_c^{(1)}(u,w), e_w \right\rangle, \tag{7.24}$$

$$\left\langle F_{c,h}^{(2)}(u^h,w^h), e_u \right\rangle = \left\langle F_{c,h}^{(2)}(u^h,w^h) - F_c^{(2)}(u,w), e_u \right\rangle, \tag{7.25}$$

which implies

$$\left\langle F_{c,h}^{(1)}(u^h,w^h), e_w \right\rangle = \tau(\nabla e_w, \nabla e_w) + (r_h^{(1)}, e_w)^h - (r^{(1)}, e_w), \tag{7.26}$$

$$\left\langle F_{c,h}^{(2)}(u^h,w^h), e_u \right\rangle = \gamma(\nabla e_u, \nabla e_u) + (r_h^{(2)}, e_u)^h - (r^{(2)}, e_u). \tag{7.27}$$

Further we have

$$(r_h^{(1)}, e_w)^h - (r^{(1)}, e_w) = (r_h^{(1)}, e_w)^h - (r_h^{(1)}, e_w) + (e_u, e_w) \tag{7.28}$$

$$\begin{aligned} (r_h^{(2)}, e_u)^h - (r^{(2)}, e_u) &= (r_h^{(2)}, e_u)^h - (r_h^{(2)}, e_u) - (e_w, e_u) \\ &\quad + (\pi_h(\lambda_c(u^h)) - \lambda_c(u^h), e_u) + (\lambda_c(u^h) - \lambda_c(u), e_u). \end{aligned} \tag{7.29}$$

One readily verifies the estimates

$$(\max(0,s) - \max(0,t))(s-t) \geq (\max(0,s) - \max(0,t))^2, \tag{7.30}$$

$$(\min(0,s) - \min(0,t))(s-t) \geq (\min(0,s) - \min(0,t))^2, \tag{7.31}$$

from which we obtain

$$(\lambda_c(u^h) - \lambda_c(u), e_u) \geq c^{-1}\|e_{\lambda_c^+}\|^2 + c^{-1}\|e_{\lambda_c^-}\|^2. \tag{7.32}$$

Hence, adding (7.26) and (7.27) and using (7.28), (7.29) and (7.32), we obtain

$$\mathcal{E} \leq \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3, \tag{7.33}$$

with

$$\begin{aligned} \mathcal{E} &:= c^{-1}\|e_{\lambda_c^+}\|^2 + c^{-1}\|e_{\lambda_c^-}\|^2 + \tau\|\nabla e_w\|^2 + \gamma\|\nabla e_u\|^2 \\ \mathcal{E}_1 &:= \left\langle F_{c,h}^{(1)}(u^h,w^h), e_w \right\rangle + (r_h^{(1)}, e_w) - (r_h^{(1)}, e_w)^h \\ \mathcal{E}_2 &:= \left\langle F_{c,h}^{(2)}(u^h,w^h), e_u \right\rangle + (r_h^{(2)}, e_u) - (r_h^{(2)}, e_u)^h \\ \mathcal{E}_3 &:= (\lambda_c(u^h) - \pi_h(\lambda_c(u^h)), e_u). \end{aligned}$$

We further estimate $\mathcal{E}_i$, $i = 1, 2, 3$. For this purpose, recall that for all v^h in $\mathcal{V}_h$ we have

$$\left\langle F_{c,h}^{(1)}(u^h, w^h), v^h \right\rangle = \left\langle F_{c,h}^{(2)}(u^h, w^h), v^h \right\rangle = 0, \tag{7.34}$$

and in particular

$$\left\langle F_{c,h}^{(1)}(u^h, w^h), \Pi_h e_w \right\rangle = \left\langle F_{c,h}^{(2)}(u^h, w^h), \Pi_h e_u \right\rangle = 0. \tag{7.35}$$

Therefore, we find that

$$\left\langle F_{c,h}^{(1)}(u^h, w^h), e_w \right\rangle = \left\langle F_{c,h}^{(1)}(u^h, w^h), e_w - \Pi_h e_w \right\rangle, \tag{7.36}$$

$$\left\langle F_{c,h}^{(2)}(u^h, w^h), e_u \right\rangle = \left\langle F_{c,h}^{(2)}(u^h, w^h), e_u - \Pi_h e_u \right\rangle. \tag{7.37}$$

Consequently, we get

$$\begin{aligned}
\mathcal{E}_1 &= \left\langle F_{c,h}^{(1)}(u^h, w^h), e_w - \Pi_h e_w \right\rangle + (r_h^{(1)}, e_w - \Pi_h e_w) \\
&\quad + (r_h^{(1)}, \Pi_h e_w) - (r_h^{(1)}, e_w)^h, \\
\mathcal{E}_2 &= \left\langle F_{c,h}^{(2)}(u^h, w^h), e_u - \Pi_h e_u \right\rangle + (r_h^{(2)}, e_u - \Pi_h e_u) \\
&\quad + (r_h^{(2)}, \Pi_h e_u) - (r_h^{(2)}, e_u)^h,
\end{aligned}$$

which we split according to

$$\begin{aligned}
\mathcal{E}_1 &= \mathcal{E}_1^a + \mathcal{E}_1^b + \mathcal{E}_1^c, \\
\mathcal{E}_2 &= \mathcal{E}_2^a + \mathcal{E}_2^b + \mathcal{E}_2^c,
\end{aligned}$$

with

$$\begin{array}{lllllll}
\mathcal{E}_1^a & = & \tau\left(\nabla w_h, \nabla(e_w - \Pi_h e_w)\right), & & \mathcal{E}_2^a & = & \gamma\left(\nabla u_h, \nabla(e_u - \Pi_h e_u)\right), \\
\mathcal{E}_1^b & = & (r_h^{(1)}, e_w - \Pi_h e_w), & & \mathcal{E}_2^b & = & (r_h^{(2)}, e_u - \Pi_h e_u), \\
\mathcal{E}_1^c & = & (r_h^{(1)}, \Pi_h e_w) - (r_h^{(1)}, \Pi_h e_w)^h, & & \mathcal{E}_2^c & = & (r_h^{(2)}, \Pi_h e_u) - (r_h^{(2)}, \Pi_h e_u)^h.
\end{array}$$

Using (7.17)–(7.20) and the Cauchy-Schwarz inequality it follows that

(7.38)

$$\mathcal{E}_1^a = \sum_{E \in \mathcal{E}_h} \tau([\nabla w^h \cdot \boldsymbol{\nu}_E]_E, e_w - \Pi_h e_w)_{0,E} \leq C \left(\tau^2 \sum_{E \in \mathcal{E}_h} (\eta_E^{(1)})^2 \right)^{1/2} \|\nabla e_w\|,$$

(7.39)

$$\mathcal{E}_1^b = \sum_{T \in \mathcal{T}_h} (r_h^{(1)}, e_w - \Pi_h e_w)_{0,T} \leq C \left(\sum_{T \in \mathcal{T}_h} (\eta_T^{(1)})^2 \right)^{1/2} \|\nabla e_w\|.$$

Moreover, from (7.19)–(7.20) and the following local estimate for the semi-inner product (see [31])

$$|(f^h, g^h)_{0,T}^h - (f^h, g^h)_{0,T}| \leq C h_T \|f^h\|_{0,T} \|g^h\|_{1,T} \quad \forall f^h \in \mathcal{V}_h,\, g^h \in \mathcal{V}_h,$$

we get

(7.40)
$$\mathcal{E}_1^c = \sum_{T\in\mathcal{T}_h} (r_h^{(1)}, \Pi_h e_w)_{0,T} - (r_h^{(1)}, \Pi_h e_w)_{0,T}^h \le C \left(\sum_{T\in\mathcal{T}_h} (\eta_T^{(1)})^2 \right)^{1/2} \|\nabla e_w\|.$$

Consequently, we infer

$$\mathcal{E}_1 := \mathcal{E}_1^a + \mathcal{E}_1^b + \mathcal{E}_1^c \le C \left(\sum_{T\in\mathcal{T}_h} (\eta_T^{(1)})^2 + \tau^2 \sum_{E\in\mathcal{E}_h} (\eta_E^{(1)})^2 \right)^{1/2} \|\nabla e_w\|. \tag{7.41}$$

In the same way, we find

$$\mathcal{E}_2 := \mathcal{E}_2^a + \mathcal{E}_2^b + \mathcal{E}_2^c \le C \left(\sum_{T\in\mathcal{T}_h} (\eta_T^{(2)})^2 + \gamma^2 \sum_{E\in\mathcal{E}_h} (\eta_E^{(2)})^2 \right)^{1/2} \|\nabla e_u\|. \tag{7.42}$$

Combining (7.33), (7.41) and (7.42) and using Young's inequality, we have proven the first assertion of the following proposition.

Proposition 7.1. *There exists a constant C depending only on the domain Ω and the smallest angle of the mesh $\mathcal{T}_h$ such that*

$$c^{-1}\|e_{\lambda_c^+}\|^2 + c^{-1}\|e_{\lambda_c^-}\|^2 + \tau\|\nabla e_w\|^2 + \gamma\|\nabla e_u\|^2 \le C\eta_\Omega^2, \tag{7.43}$$

with

$$\begin{aligned} \eta_\Omega^2 =& \tau^{-1} \sum_{T\in\mathcal{T}_h} (\eta_T^{(1)})^2 + \gamma^{-1} \sum_{T\in\mathcal{T}_h} (\eta_T^{(2)})^2 + \tau \sum_{E\in\mathcal{E}_h} (\eta_E^{(1)})^2 \\ &+ \gamma \sum_{E\in\mathcal{E}_h} (\eta_E^{(2)})^2 + \gamma^{-1} \sum_{T\in\mathcal{T}_h} (\eta_T^{(3)})^2. \end{aligned} \tag{7.44}$$

Moreover, η_Ω is bounded independently of c.

Proof. From the expression of η_Ω we have

$$\eta_\Omega \le \beta \left(\|\lambda_c(u^h)\| + \|\pi_h(\lambda_c(u^h))\| + \|u^h\|_{H^1(\Omega)} + \|w^h\|_{H^1(\Omega)} + 1 \right) \tag{7.45}$$

with a constant β which is independent of c. Further we have

$$0 \le \max\left(0, \left(\sum_{i=1}^N u^h(x_i)\phi_i\right) - 1\right) \le \left(\sum_{i=1}^N \max(0, u^h(x_i))\phi_i\right) - 1, \tag{7.46}$$

$$0 \ge \min\left(0, \left(\sum_{i=1}^N u^h(x_i)\phi_i\right) + 1\right) \ge \left(\sum_{i=1}^N \min(0, u^h(x_i))\phi_i\right) + 1. \tag{7.47}$$

As a consequence, we obtain

$$\|\lambda_c(u^h)\| \le \|\pi_h(\lambda_c(u^h))\| \tag{7.48}$$

and

$$\eta_\Omega \le \beta\left(\|\pi_h(\lambda_c(u^h))\| + \|u^h\|_{H^1(\Omega)} + \|w^h\|_{H^1(\Omega)} + 1\right). \tag{7.49}$$

From Proposition 6.2 it follows that η_Ω is bounded independently of c, which proves the claim. □

Remark 7.2.

- The estimate (7.43) constitutes an a posteriori error upper bound of Johnson's type [27] for (6.1)–(6.2). The extra term $\eta_T^{(3)}$ is due to the error incurred by using the finite element quantity $\pi_h(\lambda_c(u^h))$ to approximate $\lambda_c(u^h)$. Note, however, that $\eta_T^{(3)}$ contributes only in the set $\mathcal{I}(u^h)$ of elements with a discrete active-inactive interface, i.e.

$$\mathcal{I}(u^h) := \{T \in \mathcal{T}_h : \mathcal{AN}(T) \cap \mathcal{IN}(T) \neq \emptyset\}, \tag{7.50}$$

with

$$\mathcal{IN}(T) = \{x_i \in T : -1 < u^h(x_i) < 1\},$$
$$\mathcal{AN}(T) = \{x_i \in T : u^h(x_i) < -1 \text{ or } u^h(x_i) > 1\}.$$

- In numerical simulations we further estimate $\eta_T^{(3)}$ by $c\,h_T\|\nabla u_h\|_{0,T}$.

7.2. **Towards efficiency—a posteriori lower bounds.** Here we resort to the bubble function technique as proposed, e.g., in [34] in order to establish a lower bound on the error given in Proposition 7.1. In fact, let λ_T be the canonical bubble function of $T \in \mathcal{T}_h$, i.e., it is the product of the barycentric coordinates of T. Likewise we refer to λ_E as the canonical bubble function of $E \in \mathcal{E}_h$. We also introduce the mapping

$$\tilde{}: L^2(E) \longrightarrow L^2(\omega_E), \quad \widetilde{\sigma}(x) := \sigma(x_E) \quad x \in T,$$

which extends any function defined on an edge E to the pair of neighboring elements (T^+, T^-) defining $\omega_E = T^+ \cup T^-$. Here, we have $T \in \{T^+, T^-\}$, and $x_E \in E$ is such that $x - x_E$ is parallel to a fixed $E' \in T - \{E\}$. Referring to [34], for all polynomial functions $\sigma_T \in P_k(T)$ and $\sigma_E \in P_k(E)$, $k \in \mathbb{N}$, the following estimates hold true:

$$\|\sigma_T\|_{0,T}^2 \le C(\sigma_T, \sigma_T\lambda_T)_{0,T} \quad \forall T \in \mathcal{T}_h, \tag{7.51}$$

$$\|\sigma_T\lambda_T\|_{0,T} \le \|\sigma_T\|_{0,T} \quad \forall T \in \mathcal{T}_h, \tag{7.52}$$

$$|\sigma_T\lambda_T|_{1,T} \le Ch_T^{-1}\|\sigma_T\|_{0,T} \quad \forall T \in \mathcal{T}_h, \tag{7.53}$$

$$\|\sigma_E\|_{0,E}^2 \le C(\sigma_E, \sigma_E\lambda_E)_{0,E} \quad \forall E \in \mathcal{E}_h, \tag{7.54}$$

$$\|\sigma_E\lambda_E\|_{0,E} \le C\|\sigma_E\|_{0,E} \quad \forall E \in \mathcal{E}_h, \tag{7.55}$$

Furthermore, we have

$$\|\widetilde{\sigma_E}\lambda_E\|_{0,\omega_E} \le Ch_E^{1/2}\|\sigma_E\|_{0,E} \quad \forall E \in \mathcal{E}_h, \tag{7.56}$$

$$|\widetilde{\sigma_E}\lambda_E|_{1,\omega_E} \le Ch_E^{-1/2}\|\sigma_E\|_{0,E} \quad \forall E \in \mathcal{E}_h. \tag{7.57}$$

Our main theorem relies on the following two auxiliary results.

Lemma 7.3. *For every $T \in \mathcal{T}_h$, there hold*

$$\tau^{-1}(\eta_T^{(1)})^2 \leq C\left(\tau|e_w|_{1,T}^2 + \tau^{-1}\|h_T e_u\|_{0,T}^2 + \tau^{-1} osc^2(r_h^{(1)}, T)\right) \tag{7.58}$$

and

$$\begin{aligned}\gamma^{-1}(\eta_T^{(2)})^2 \leq & C\left(\gamma|e_u|_{1,T}^2 + \gamma^{-1}\|h_T e_w\|_{0,T}^2 + \gamma^{-1}\|h_T e_{\lambda_c^+}\|_{0,T}^2\right.\\ &\left. + \gamma^{-1}\|h_T e_{\lambda_c^-}\|_{0,T}^2 + \gamma^{-1}\|h_T e_{\lambda_c^h}\|_{0,T}^2 + \gamma^{-1} osc^2(r_h^{(2)}, T)\right).\end{aligned} \tag{7.59}$$

Proof. We have

$$(\eta_T^{(2)})^2 = \|h_T r_h^{(2)}\|_{0,T}^2 \leq 2h_T^2\|\overline{r}_h^{(2)}\|_{0,T}^2 + 2\mathrm{osc}_h(r_h^{(2)}, T)^2, \tag{7.60}$$

with $\overline{r}_h^{(2)} := \overline{\pi_h(\lambda_c(u^h))} - \overline{w}_h - \overline{u}_{old}$. By setting $\psi_T := \overline{r}_h^{(2)}|_T \lambda_T$ and using (7.51) we get

$$\|\overline{r}_h^{(2)}\|_{0,T}^2 \leq C(\overline{r}_h^{(2)}, \psi_T)_{0,T}$$

and further

$$\|\overline{r}_h^{(2)}\|_{0,T}^2 \leq C(r_h^{(2)}, \psi_T)_{0,T} + Ch_T^{-1}\mathrm{osc}_h(r_h^{(2)}, T)\|\psi_T\|_{0,T}. \tag{7.61}$$

Since $\Delta u^h|_T = 0$ and $-\gamma\Delta u + \lambda_c(u) - w - u_{old} = 0$, we have

$$\begin{aligned}(r_h^{(2)}, \psi_T)_{0,T} &= \gamma(\nabla e_u, \nabla\psi_T)_{0,T} - (e_w, \psi_T)_{0,T} + (\pi_h(\lambda_c(u^h)) - \lambda_c(u), \psi_T)_{0,T}\\ &= \gamma(\nabla e_u, \nabla\psi_T)_{0,T} - (e_w, \psi_T)_{0,T}\\ &\quad + (\pi_h(\lambda_c(u^h)) - \lambda_c(u^h), \psi_T)_{0,T} + (\lambda_c(u^h) - \lambda_c(u), \psi_T)_{0,T}\\ &= \gamma(\nabla e_u, \nabla\psi_T)_{0,T} - (e_w, \psi_T)_{0,T}\\ &\quad + (e_{\lambda_c^h}, \psi_T)_{0,T} + (e_{\lambda_c^+}, \psi_T)_{0,T} + (e_{\lambda_c^-}, \psi_T)_{0,T}.\end{aligned} \tag{7.62}$$

From (7.61)–(7.62) it follows that

$$\begin{aligned}\|\overline{r}_h^{(2)}\|_{0,T}^2 \leq C\Big(&\gamma|e_u|_{1,T}|\psi_T|_{1,T} + \Big(\|e_w\|_{0,T} + \|e_{\lambda_c^h}\|_{0,T} + \|e_{\lambda_c^+}\|_{0,T}\\ &+ \|e_{\lambda_c^-}\|_{0,T} + h_T^{-1}\mathrm{osc}_h(r_h^{(2)}, T)\Big)\|\psi_T\|_{0,T}\Big),\end{aligned}$$

and using (7.52) and (7.53) we obtain

$$\begin{aligned}\|\overline{r}_h^{(2)}\|_{0,T} \leq C\Big(&\gamma h_T^{-1}|e_u|_{1,T} + \|e_w\|_{0,T} + \|e_{\lambda_c^h}\|_{0,T}\\ &+ \|e_{\lambda_c^+}\|_{0,T} + \|e_{\lambda_c^-}\|_{0,T} + h_T^{-1}\mathrm{osc}_h(r_h^{(2)}, T)\Big).\end{aligned} \tag{7.63}$$

The estimation (7.59) now follows from (7.60) and (7.63).

Using similar argument one can show (7.58). □

Lemma 7.4. *For every $E \in \mathcal{E}_h$ there hold*

$$\tau(\eta_E^{(1)})^2 \leq C\left(\tau|e_w|_{1,\omega_E}^2 + \tau^{-1}\|h_E e_u\|_{0,\omega_E}^2 + \tau^{-1} osc^2(r_h^{(1)}, \omega_E)\right) \tag{7.64}$$

and

(7.65)

$$\gamma(\eta_E^{(2)})^2 \le C\Big(\gamma|e_u|^2_{1,\omega_E} + \gamma^{-1}\|h_E e_w\|^2_{0,\omega_E} + \gamma^{-1}\|h_E e_{\lambda_c^+}\|^2_{0,\omega_E}$$
$$+\gamma^{-1}\|h_E e_{\lambda_c^-}\|^2_{0,\omega_E} + \gamma^{-1}\|h_E e_{\lambda_c^h}\|^2_{0,\omega_E} + \gamma^{-1} osc^2(r_h^{(2)},\omega_E)\Big).$$

Proof. Let E be an arbitrary edge in $\mathcal{E}^h$ and define $\psi_E := \widetilde{\sigma_E}\lambda_E$ with $\sigma_E := [\nabla u^h]_E \cdot \boldsymbol{\nu}_E$. Due to (7.54) we have

$$(\eta_E^{(2)})^2 := h_E\|[\nabla u^h]_E \cdot \boldsymbol{\nu}_E\|^2_{0,E} \le C h_E([\nabla u^h]_E \cdot \boldsymbol{\nu}_E, \psi_E)_{0,E}.$$

Green's formula and $\Delta u^h|_T = 0$ yield

$$([\nabla u^h]_E \cdot \boldsymbol{\nu}_E, \psi_E)_{0,E} = \sum_{T\subset\omega_E} (\nabla u^h, \nabla\psi_E)_{0,T}.$$

Using $-\gamma\Delta u + \lambda_c(u) - w - u_{old} = 0$ we get

$$\begin{aligned}
([\nabla u^h]_E \cdot \boldsymbol{\nu}_E, \psi_E)_{0,E} &= (\nabla e_u, \nabla\psi_E)_{0,\omega_E} - \gamma^{-1}(e_w,\psi_E)_{0,\omega_E} \\
&\quad +\gamma^{-1}(\pi_h(\lambda_c(u^h)) - \lambda_c(u), \psi_E)_{0,\omega_E} \\
&\quad -\gamma^{-1}(r_h^{(2)}\psi_E)_{0,\omega_E} \\
&= (\nabla e_u, \nabla\psi_E)_{0,\omega_E} - \gamma^{-1}(e_w,\psi_E)_{0,\omega_E} \\
&\quad +\gamma^{-1}(\pi_h(\lambda_c(u^h)) - \lambda_c(u^h), \psi_E)_{0,\omega_E} \\
&\quad +\gamma^{-1}(\lambda_c(u^h) - \lambda_c(u), \psi_E)_{0,\omega_E} - \gamma^{-1}(r_h^{(2)},\psi_E)_{0,\omega_E} \\
&= (\nabla e_u, \nabla\psi_E)_{0,\omega_E} - \gamma^{-1}(e_w,\psi_E)_{0,\omega_E} \\
&\quad +\gamma^{-1}(e_{\lambda_c^h},\psi_E)_{0,\omega_E} + \gamma^{-1}(e_{\lambda_c^+},\psi_E)_{0,\omega_E} \\
&\quad +\gamma^{-1}(e_{\lambda_c^-},\psi_E)_{0,\omega_E} - \gamma^{-1}(r_h^{(2)},\psi_E)_{0,\omega_E}.
\end{aligned}$$

Consequently, we obtain

$$\begin{aligned}
([\nabla u^h]_E \cdot \boldsymbol{\nu}_E, \psi_E)_{0,E} \le{}& \|\nabla e_u\|_{0,\omega_E}\|\nabla\psi_E\|_{0,\omega_E} + \gamma^{-1}\|e_w\|_{0,\omega_E}\|\psi_E\|_{0,\omega_E} \\
&+ \gamma^{-1}\|e_{\lambda_c^h}\|_{0,\omega_E}\|\psi_E\|_{0,\omega_E} + \gamma^{-1}\|e_{\lambda_c^+}\|_{0,\omega_E}\|\psi_E\|_{0,\omega_E} \\
&+ \gamma^{-1}\|e_{\lambda_c^-}\|_{0,\omega_E}\|\psi_E\|_{0,\omega_E} + \gamma^{-1}\|r_h^{(2)}\|_{0,\omega_E}\|\psi_E\|_{0,\omega_E}.
\end{aligned}$$

Using (7.54), (7.56) and (7.57), it follows that

$$\|[\nabla u^h]_E \cdot \boldsymbol{\nu}_E\|^2_{0,E} \le C([\nabla u^h]_E \cdot \boldsymbol{\nu}_E, \psi_E)_{0,E}$$

and

$$\begin{aligned}
\|[\nabla u^h]_E \cdot \boldsymbol{\nu}_E\|_{0,E} \le C\Big(& h_E^{-1/2}\|\nabla e_u\|_{0,\omega_E} + \gamma^{-1}h_E^{1/2}\|e_w\|_{0,\omega_E} \\
&+ \gamma^{-1}h_E^{1/2}\|e_{\lambda_c^h}\|_{0,\omega_E} + \gamma^{-1}h_E^{1/2}\|e_{\lambda_c^+}\|_{0,\omega_E} \\
&+\gamma^{-1}h_E^{1/2}\|e_{\lambda_c^-}\|_{0,\omega_E} + \gamma^{-1}h_E^{1/2}\|r_h^{(2)}\|_{0,\omega_E}\Big).
\end{aligned}$$

Therefore, we have

$$
\begin{aligned}
\gamma(\eta_E^{(2)})^2 &:= \gamma h_E \|[\nabla e^h]_E \cdot \boldsymbol{\nu}_E\|_{0,E}^2 \\
&\le C\Big(\gamma |e_u|_{1,\omega_E}^2 + \gamma^{-1}\|h_E e_w\|_{0,\omega_E}^2 + \gamma^{-1}\|h_E e_{\lambda_c^+}\|_{0,\omega_E}^2 \\
&\quad + \gamma^{-1}\|h_E e_{\lambda_c^-}\|_{0,\omega_E}^2 + \gamma^{-1}\|h_E e_{\lambda_c^h}\|_{0,\omega_E}^2 + \gamma^{-1}\|h_E r_h^{(2)}\|_{0,\omega_E}\Big).
\end{aligned}
\tag{7.66}
$$

Observe that due to (7.11) it holds that

$$
\gamma^{-1}\|h_E r_h^{(2)}\|_{0,\omega_E}^2 \le C \sum_{T\in\omega_E} \gamma^{-1}(\eta_T^{(2)})^2, \tag{7.67}
$$

where the regularity of the mesh, i.e. $\mathcal{O}(h_E/h_T) = 1$, is used. Consequently by combining (7.59), (7.66) and (7.67) we obtain (7.65).

The estimation (7.64) can be shown in an analogous way. □

Using the two previous lemmas we easily obtain the following global posteriori lower bound.

Proposition 7.5. *There exists a constant β depending on c^{-1}, γ, τ, Ω, and the smallest angle of the mesh $\mathcal{T}_h$ such that*

$$
\begin{aligned}
c^{-1}\|e_{\lambda_c^+}\|^2 + c^{-1}\|e_{\lambda_c^-}\|^2 + \tau\|\nabla e_w\|^2 + \gamma\|\nabla e_u\|^2 \ge \\
\beta\eta_\Omega^2 - \|e_{\lambda_c^h}\|^2 - osc_h(r_h^{(1)},\Omega)^2 - osc_h(r_h^{(2)},\Omega)^2.
\end{aligned}
\tag{7.68}
$$

Remark 7.6. If the discrete set $\mathcal{I}(u^h)$ is empty or when the lumping technique is replaced by an exact computation of $\max(0, u^h - 1)$ and $\min(0, u^h + 1)$, then $\|e_{\lambda_c^h}\| = 0$ and one gets a global lower estimate for η_Ω which depends on c^{-1} through β. Note, however, that in these cases and for fixed c our estimator is both reliable and efficient.

7.3. **Mesh adaptation.** The marking of elements for a possible refinement or coarsening, respectively, is based on a bulk-type criterion; see [16] for the latter. For this purpose, for a given triangulation $\mathcal{T}_h$ we introduce the set

$$
\mathcal{A}_h := \{T \in \mathcal{T}_h : \alpha_{\min} \le |T| \le \alpha_{\max}\},
$$

with $0 \le \alpha_{\min} < \alpha_{\max}$ denoting the admissible minimal and maximal element areas, respectively. The corresponding marking algorithm performs the following steps:

(1) Fix constants θ^r and θ^c in $]0,1[$.

(2) Find a set $\mathcal{M}_h^T \subset \mathcal{T}_h$ such that

$$
\sum_{T\in\mathcal{M}_h^T} \Big(\tau^{-1}(\eta_T^{(1)})^2 + \gamma^{-1}(\eta_T^{(2)})^2\Big) \ge \theta^r \sum_{T\in\mathcal{T}_h} \Big(\tau^{-1}(\eta_T^{(1)})^2 + \gamma^{-1}(\eta_T^{(2)})^2\Big).
$$

(3) Find a set $\mathcal{M}_h^E \subset \mathcal{T}_h$ such that

$$
\sum_{T\in\mathcal{M}_h^E} \sum_{E\in\mathcal{E}_h(T)} \Big(\tau(\eta_E^{(1)})^2 + \gamma(\eta_E^{(2)})^2\Big) \ge \theta^r \sum_{T\in\mathcal{T}_h} \sum_{E\in\mathcal{T}_h} \Big(\tau(\eta_E^{(1)})^2 + \gamma(\eta_E^{(2)})^2\Big).
$$

(4) Find a set $\mathcal{M}_h^\lambda \subset \mathcal{T}_h \cap \mathcal{I}(u^h)$ such that

$$\sum_{T\in\mathcal{M}_h^\lambda} \gamma^{-1}(\eta_T^{(3)})^2 \geq \theta^r \sum_{T\in\mathcal{T}_h\cap\mathcal{I}(u^h)} \gamma^{-1}(\eta_T^{(3)})^2.$$

(5) Mark each $T \in (\mathcal{M}_h^E \cup \mathcal{M}_h^T \cup \mathcal{M}_h^\lambda) \cap \mathcal{A}_h$ for refinement.

(6) Find the set $\mathcal{C}_h^T \subset \mathcal{T}_h$ such that

$$\tau^{-1}(\eta_T^{(1)})^2 + \gamma^{-1}(\eta_T^{(2)})^2 \leq \frac{\theta^c}{N_T} \sum_{T\in\mathcal{T}_h} \left(\tau^{-1}(\eta_T^{(1)})^2 + \gamma^{-1}(\eta_T^{(2)})^2\right)$$

for each $T \in \mathcal{C}_h^T$. Here and below N_T denotes the number of elements of $\mathcal{T}_h$.

(7) Find the set $\mathcal{C}_h^E \subset \mathcal{T}_h$ such that

$$\sum_{E\in\mathcal{E}_h(T)} \tau(\eta_E^{(1)})^2 + \gamma(\eta_E^{(2)})^2 \leq \frac{\theta^c}{N_T} \sum_{T\in\mathcal{T}_h} \sum_{E\in\mathcal{E}_h(T)} \left(\tau(\eta_E^{(1)})^2 + \gamma(\eta_E^{(2)})^2\right)$$

for each $T \in \mathcal{C}_h^E$.

(8) Find the set $\mathcal{C}_h^\lambda \subset \mathcal{T}_h \cap \mathcal{I}(u^h)$ such that

$$\gamma^{-1}(\eta_T^{(3)})^2 \leq \frac{\theta^c}{N_T} \sum_{T\in\mathcal{T}_h\cap\mathcal{I}(u^h)} \gamma^{-1}(\eta_T^{(3)})^2.$$

for each $T \in \mathcal{C}_h^\lambda \cap \mathcal{I}(u^h)$.

(9) Mark all $T \in \left(\mathcal{C}_h^T \cup \mathcal{C}_h^E \cup \mathcal{C}_h^\lambda\right) \cap \mathcal{A}_h$ for coarsening.

Note that flagging elements for refinement (resp. coarsening) is done in the three separate steps (2)-(4) (resp. (5)-(7)). This has the advantage of properly handling the scaling difference between jump, element and interpolation residual contributions induced by τ and γ in (7.43). We further mention that within one mesh adaptation step, an element T might be subject to both refinement and coarsening.

Given a mesh at a current time instance in the context of the time-dependent Cahn-Hilliard problem, we use the above marking strategy once to produce a new mesh for the next time step. This yields the following overall adaptive algorithm:

(1) Determine an initial mesh $\mathcal{T}_h^{(0)}$ and an initial $u^h(0)$. Set $i = 0$.
(2) Denote by t_{i+1} the current time instance.
(3) For each $T \in \mathcal{T}_h^i$ and $E \in \mathcal{E}_h^j$, compute the posteriori local error estimates $\eta_T^{(i)}$ and $\eta_E^{(j)}$ for $i = 1, \ldots, 3$ and $j = 1, 2$.
(4) For each $T \in \mathcal{T}_h^i$ (resp. $E \in \mathcal{E}_h^i$), mark T (resp. E) for refinement/coarsening using the bulk criterion.
(5) Refine/coarse mesh to obtain a new mesh denoted by $\mathcal{T}_h^{(i+1)}$ and perform a time step.

Our strategy is motivated by the fact that the time step τ should be chosen sufficiently small to capture the fast dynamics at the beginning of the evolution. For $\tau = \mathcal{O}(\gamma)$, this strategy has performed well in our numerical experiments.

8. Numerical results

In this section we assess the practical performance of the proposed AFEM Moreau-Yosida-based (or equivalently semi-smooth-Newton) algorithm. For this purpose, a Matlab code was written using coarsening/refinement routines of the iFEM finite elements library [9]. All computations were carried out on a Linux workstation with two duo-core Intel-Xeon 3 GHz processors and 4GB of RAM.

In the experiments reported on below we have $\Omega =]0,1[^2$. The handling of the parameter c is as follows: For the first time instance and since the initial solution might not be a good starting point for the semi-smooth Newton method, a continuation procedure is used with respect to c, i.e. (6.1)–(6.2) is solved for a sequence of increasing c-values. In fact, we take $c_1 = 10 \leq c_2 = 10^2 \leq \cdots \leq c_7 = 10^7 = c_{max}$. The Newton method for solving the system for c_{i+1} is initialized by an approximate solution for c_i. We note that more sophisticated c-update strategies may be employed; compare [24, 25]. For the subsequent time steps, $c = c_{max} = 10^7$ is fixed. This is appropriate due to the rather small time step size. For solving the linear systems involved in the semi-smooth-Newton method we use BICGSTAB with super-LU preconditioning [14]. The Newton solver was stopped as soon as

$$\|F_c(u_h^{(k)}, w_h^{(k)})\|_2 \leq \epsilon_{\text{rel}} \|F_c(u_h^{(0)}, w_h^{(0)})\|_2 + \epsilon_{\text{abs}}, \quad k = 1 \ldots k_{max},$$

for some user-specified maximum number of iterations k_{max} and tolerances ϵ_{rel} and ϵ_{abs}. In our tests we used

$$k_{max} = 100, \quad \epsilon_{\text{rel}} = 10^{-12}, \quad \epsilon_{\text{abs}} = 10^{-6}.$$

We note that the method converged within at most 5 iterations at every time instance.

Example 1. In our first example we consider the initial order parameter u_0 given by

$$\begin{aligned} u_0(x,y) = {} & \tanh\left(((x-0.3)^2 + (y-0.5)^2 - 0.14^2)/\varepsilon\right) \\ & \times \tanh\left(((x-0.7)^2 + (y-0.5)^2 - 0.24^2)/\varepsilon\right), \end{aligned}$$

which encloses two circles of centers $(0.3, 0.5)$ and $(0.7, 0.5)$ and radius 0.14 and 0.24, respectively. We set $\varepsilon = 10^{-3}$, $\tau = 10^{-4}$ and $\pi\gamma = 10^{-3}$. For the mesh adaptation process, $\theta_T^r = 0.6$ and $\theta^c = 0.1$ are fixed. Initially a uniform mesh of 32768 elements and 16641 nodes is selected.

In Figures 8.1–8.4 we depict snapshots of the order parameter u and the corresponding mesh at different time steps during the numerical solution process. One clearly observes how the mesh refinement follows the transition zone. The minimum element area 5×10^{-6} is reached in almost all time steps which indicates that one would need 5×10^6 elements if a uniform mesh were used. As expected, in Figure 8.5 the free energy is reduced in time.

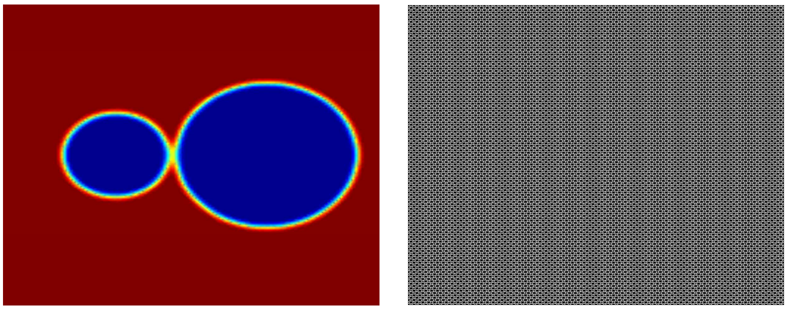

FIGURE 8.1. Order parameter u at time $t = 0\tau$ and corresponding uniform mesh with 32768 elements and 16641 nodes.

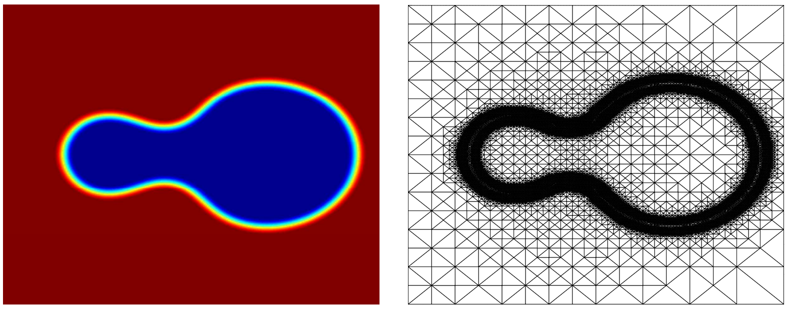

FIGURE 8.2. Order parameter u at time $t = 100\tau$ and corresponding mesh with 36532 elements and 18294 nodes.

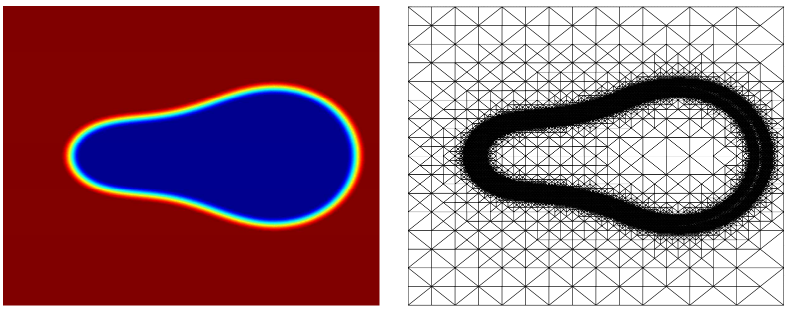

FIGURE 8.3. Order parameter u at time $t = 500\tau$ and corresponding mesh with 35230 elements and 17645 nodes.

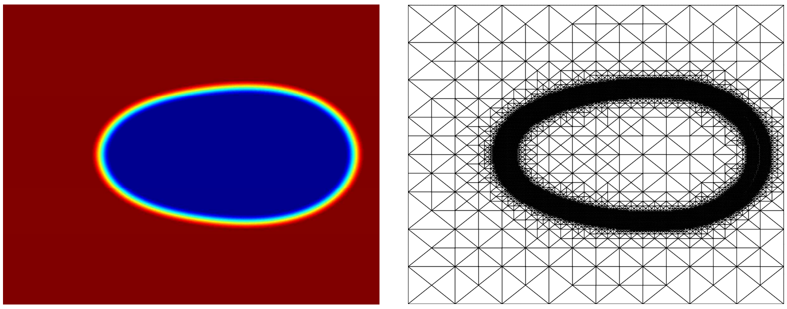

FIGURE 8.4. Order parameter u at time $t = 2000\tau$ and corresponding mesh with 33282 elements and 16663 nodes.

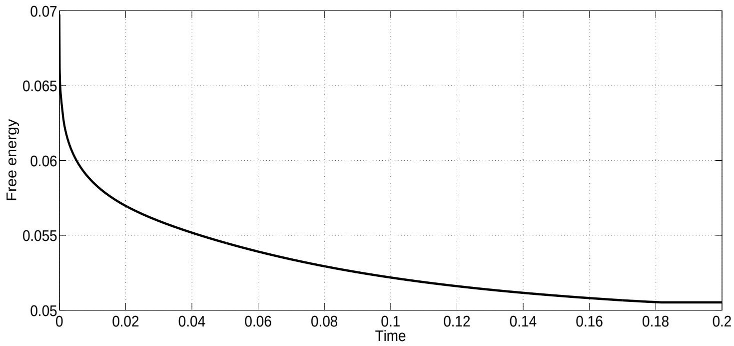

FIGURE 8.5. Free energy versus time.

Example 2: Spinodal decomposition. Now we consider the case of spinodal decomposition in two spatial dimensions. In this case, the initial data is a random perturbation of magnitude 0.05 about a mean composition of 0. We take $\pi\gamma = 10^{-3}$ and $\tau = 5 \times 10^{-4}$. For the mesh adaptation process, we choose $\theta^r = 0.6$ and $\theta^c = 0.2$.

In Figures 8.6–8.9, as before we depict snapshots of the order parameter u and the corresponding mesh at different time steps along the numerical solution. The initial uniform mesh is chosen with 32768 elements and 16641 nodes. As in the previous example, the minimum element area is set to 5×10^{-6}. Typically, the minimal area is reached in almost every time instance indicating that a uniform mesh refinement would yield 5×10^{6} elements. The free-energy decrease in time as shown in Figure 8.10. In the same figure we also monitor the evolution in time of the number of degrees of freedom. As expected for the spinodal decomposition we get finer meshes in the first few steps. Once phase regions alternating between the two components form, the effect of refinement/coarsening gets increasingly more pronounced: the refinement zone follows the transition layer throughout the time interval (see Figures 8.6–8.9).

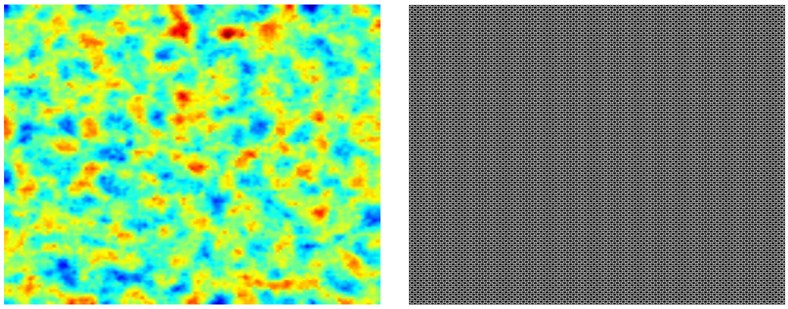

FIGURE 8.6. Order parameter u at time $t = 0$ and corresponding mesh with 32768 elements and 16641 nodes.

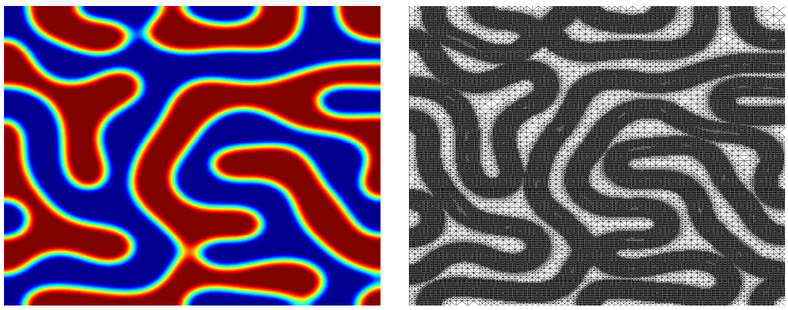

FIGURE 8.7. Order parameter u at time $t = 50\tau$ and corresponding mesh with 129684 elements and 65085 nodes.

APPENDIX: MATHEMATICAL PROGRAMMING IN BANACH SPACE

In this section we recall the mathematical programming theory in Banach space as given by Zowe and Kurcyusz in [33].

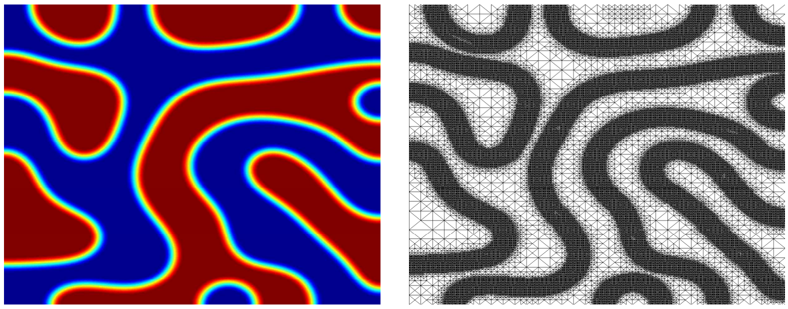

FIGURE 8.8. Order parameter u at time $t = 100\tau$ and corresponding mesh with 100513 elements and 50454 nodes.

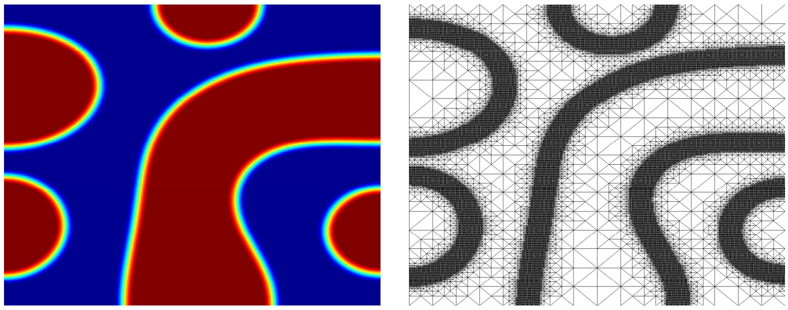

FIGURE 8.9. Order parameter u at time $t = 500\tau$ and corresponding mesh with 55482 elements and 27850 nodes.

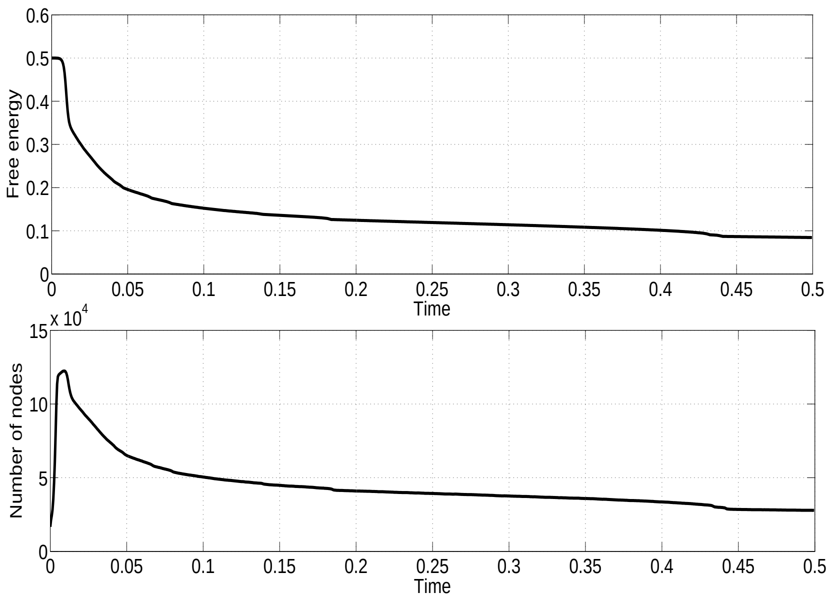

FIGURE 8.10. Free energy and number of nodes versus time.

Let $\mathcal{X}$ and $\mathcal{Y}$ be real Banach spaces. For

$$\begin{array}{rclr} F:\mathcal{X} & \longrightarrow & \mathbb{R} & \text{Fréchet-differentiable,} \\ g:\mathcal{X} & \longrightarrow & \mathcal{Y} & \text{continuously Fréchet-differentiable,} \end{array}$$

we consider the following mathematical program:

$$\min\left\{F(x)\ \mid g(x)\in M,\ x\in C\right\}, \tag{8.1}$$

where C is a convex closed subset of $\mathcal{X}$ and M a closed cone in $\mathcal{Y}$ with vertex at 0. We suppose that (8.1) has an optimal solution $\hat{x}$, and introduce the conical hulls of $C-\{\hat{x}\}$ and $M-\{y\}$, respectively, as

$$\begin{array}{rcl} C(\hat{x}) & = & \{x\in\mathcal{X}\mid \exists\beta\geq 0,\,\exists c\in C,\ x=\beta(c-\hat{x})\}, \\ M(y) & = & \{z\in\mathcal{Y}\mid \exists\lambda\geq 0,\,\exists\zeta\in M,\ z=\zeta-\lambda y\}. \end{array}$$

Then the main result in [33] on the existence of a Lagrange multiplier for (8.1) is as follows.

Theorem 8.1. *Let $\hat{x}$ be an optimal solution of the problem* (8.1) *satisfying the following constraints qualification:*

$$g'(\hat{x})\cdot C(\hat{x})-M(g(\hat{x}))=\mathcal{Y}. \tag{8.2}$$

Then there exists a Lagrange multiplier $\mu^*\in\mathcal{Y}^*$ such that

$$\langle\mu^*,\,z\rangle_{\mathcal{Y}^*,\mathcal{Y}} \geq 0 \quad \forall z\in M, \tag{8.3}$$

$$\langle\mu^*,\,g(\hat{x})\rangle_{\mathcal{Y}^*,\mathcal{Y}} = 0, \tag{8.4}$$

$$F'(\hat{x})-\mu^*\circ g'(\hat{x}) \in C(\hat{x})_+, \tag{8.5}$$

where $A_+=\left\{x^*\in\mathcal{X}^*:\ \langle x^*,\,a\rangle_{\mathcal{X}^*,\mathcal{X}}\geq 0\ \forall a\in A\right\}$, $\mathcal{Y}^*$ and $\mathcal{X}^*$ are the topological dual spaces of $\mathcal{Y}$ and $\mathcal{X}$, respectively, and $(\mu^*\circ g'(\hat{x}))\,d=\langle\mu^*,\,g'(\hat{x})\ d\rangle_{\mathcal{Y}^*,\mathcal{Y}}$ $\forall d\in\mathcal{X}$.

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