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OPTIMAL CONTROL OF TIME-DISCRETE TWO-PHASE FLOW DRIVEN BY A DIFFUSE-INTERFACE MODEL *

Harald Garcke[1], Michael Hinze[2] and Christian Kahle[3]

Abstract. We propose a general control framework for two-phase flows with variable densities in the diffuse interface formulation, where the distribution of the fluid components is described by a phase field. The flow is governed by the diffuse interface model proposed in [Abels, Garcke, Grün, M3AS 22(3):1150013(40), 2012]. On the basis of the stable time discretization proposed in [Garcke, Hinze, Kahle, APPL NUMER MATH, 99:151–171, 2016] we derive necessary optimality conditions for the time-discrete and the fully discrete optimal control problem. We present numerical examples with distributed and boundary controls, and also consider the case, where the initial value of the phase field serves as control variable.

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1. Introduction

In this paper we study a general discrete framework for control of two-phase fluids governed by the thermodynamically consistent diffuse interface model proposed in [5]. For the discretization we use the approach of [23], where the authors propose a time discretization scheme, that preserves this important property in the time discrete setting and, using a post-processing step, also in the fully discrete setting including adaptive mesh discretization. As control actions we consider distributed control, Dirichlet boundary control, and control with the initial condition of the phase field.

For the practical implementation we adapt the adaptive treatment developed in [23] to the optimal control setting. On the discrete level, special emphasis has to be be taken for the control with the intial value of the phase field, since the distribution of its phases is an outcome of the optimization procedure and thus a-priori

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unknown. In this case we combine the variational discretization from [38] with error estimation techniques to find a good mesh for the numerical representation of the a-priori unknown phase distribution.

Let us comment on related literature on time discretizations and control of (two-phase) fluids. For investigations of further time discretizations we refer to [7, 23, 27–29, 31, 34]. Concerning optimal control and feedback control of fluids there is a wide range of literature available. Here we only mention [13, 14, 22, 30, 37, 40].

Let us further comment on available literature for control of Cahn–Hilliard multiphase flow systems. In [35] distributed optimal control of the Cahn–Hilliard system with a non smooth double obstacle potential is proposed, and in [36] this work is extended to time-discrete two-phase flow given by a Cahn–Hilliard Navier–Stokes system with equal densities. Both works aim at existence of optimal controls and first order optimality conditions. In [34] the authors consider time discrete optimal control of multiphase flows based on the diffuse interface model of [5]. This work aims at establishing existence of solutions and stationarity conditions for control problems with free energies governed by the double obstacle potential, which is achieved through an appropriate limiting process of control problems with smooth relaxed free energies. In [32] a goal oriented adaptive concept for the numerical realization is proposed. The focus of the present work is different in that we consider numerical analysis of the fully discrete problem, propose a tailored numerical adaptive concept for the control problem, and present numerical examples which clearly show the potential of our approach.

We also mention the work of [12], where optimal control for a binary fluid, that is described by its density distribution, is proposed.

Let us finally comment on feedback control approaches for multiphase flows. Model predictive control is applied to the model from [5] in [39, 43, 44].

The paper is organized as follows. In Section 2 we state the model for the two-phase system and summarize assumptions that we require for the data. In Section 3 we state the time discretization scheme proposed in [23] and summarize properties of the scheme which we need in the present paper. We formulate the time discrete optimization problem in Section 3. In Section 4 we consider the optimal control problem in the fully discrete setting and present numerical examples in Section 6.

2. The governing equations

The two-phase flow is modeled by the diffuse interface model proposed in [5].

$$\begin{aligned}
\rho\partial_t v + ((\rho v + j)\cdot\nabla)\, v - \operatorname{div}(2\eta D v) + \nabla\pi & \\
-\mu\nabla\varphi - \rho K - f &= 0 && \forall x\in\Omega,\ \forall t\in I, && (1)\\
-\operatorname{div}(v) &= 0 && \forall x\in\Omega,\ \forall t\in I, && (2)\\
\partial_t\varphi + v\cdot\nabla\varphi - b\Delta\mu &= 0 && \forall x\in\Omega,\ \forall t\in I, && (3)\\
-\sigma\epsilon\Delta\varphi + \frac{\sigma}{\epsilon}W'(\varphi) - \mu &= 0 && \forall x\in\Omega,\ \forall t\in I, && (4)\\
v(0,x) &= v_0(x) && \forall x\in\Omega, && (5)\\
\varphi(0,x) &= \varphi_0(x) && \forall x\in\Omega, && (6)\\
v(t,x) &= g && \forall x\in\partial\Omega,\ \forall t\in I, && (7)\\
\nabla\mu(t,x)\cdot\nu_\Omega = \nabla\varphi(t,x)\cdot\nu_\Omega &= 0 && \forall x\in\partial\Omega,\ \forall t\in I. && (8)
\end{aligned}$$

Here φ denotes the phase field, μ the chemical potential, v the velocity field and π the pressure. Furthermore $j = -\frac{\rho_2-\rho_1}{2}b\nabla\mu$ is a diffuse flux for φ.

In addition $\Omega\subset\mathbb{R}^n, n\in\{2,3\}$, denotes an open, convex and polygonal ($n=2$) or polyhedral ($n=3$) bounded domain. In particular it has Lipschitz boundary. Convexity of the domain is needed as we use H^2-regularity results for Poisson's equation with L^2 right hand sides which hold in polygonal or polyhedral domains if the domain is convex. Its outer unit normal is denoted as ν_Ω, and $I = (0,T]$ with $0 < T < \infty$ is a time interval.

The free energy density is denoted by W and is assumed to be of double-well type with exactly two minima at ± 1. For W we use a splitting $W = W_+ + W_-$, where W_+ is convex and W_- is concave.

The density is denoted by $\rho = \rho(\varphi)$, fulfilling $\rho(-1) = \rho_1$ and $\rho(1) = \rho_2$, where ρ_1, ρ_2 denote the densities of the involved fluids. The viscosity is denoted by $\eta = \eta(\varphi)$, fulfilling $\eta(-1) = \eta_1$ and $\eta(1) = \eta_2$, with individual fluid viscosities η_1, η_2. The constant mobility is denoted by b, but this work can be generalized to general non-degenerate mobilites. The gravitational force is denoted by K. By $Dv = \frac{1}{2}\left(\nabla v + (\nabla v)^t\right)$ we denote the symmetrized gradient. The scaled surface tension is denoted by $\sigma > 0$ and the interfacial width is proportional to $\epsilon > 0$ which is fixed throughout this work. We further have a volume force f and boundary data g, as well as an initial phase field φ_0 and a solenoidal initial velocity field v_0.

Concerning results on existence of solutions for (1)–(8) under different assumptions on W and b we refer to [3, 4, 26].

Assumptions

For the data of our problem we assume:

(A1) $W : \mathbb{R} \to \mathbb{R}$ is twice continuously differentiable and is of double-well type, i.e. it has exactly two minima at ± 1 with values $W(\pm 1) = 0$.

(A2) W_+' and W_-' are Frechét differentiable as operators from $H^1(\Omega)$ to $(H^1(\Omega))^\star$. Furthermore $(W_+''(\xi)\delta\varphi, \delta\varphi) \geq 0$ holds for all $\xi, \delta\varphi \in H^1(\Omega)$.

(A3) W and its derivatives are polynomially bounded, i.e. there exists a $C > 0$ such that $|W(x)| \leq C(1+|x|^q)$, $|W_+'(x)| \leq C(1+|x|^{q-1})$, $|W_-'(x)| \leq C(1+|x|^{q-1})$, $|W_+''(x)| \leq C(1+|x|^{q-2})$, and $|W_-''(x)| \leq C(1+|x|^{q-2})$ holds for some $q \in [2,4]$ if $n = 3$ and $q \in [2,\infty)$ if $n = 2$.

(A4) There exists $\varphi_a \leq -1$ and $\varphi_b \geq 1$, such that $\rho(\varphi) = \rho(\varphi_a)$ for $\varphi \leq \varphi_a$, and $\rho(\varphi) = \rho(\varphi_b)$ for $\varphi \geq \varphi_b$. For $\varphi_a < \varphi < \varphi_b$ the function $\rho(\varphi)$ is affine linear, i.e. $\rho(\varphi) = \frac{1}{2}\left((\rho_2 - \rho_1)\varphi + (\rho_1 + \rho_2)\right)$, and we define $\rho_\delta := \frac{(\rho_2 - \rho_1)}{2}$.

Further, $\eta(\varphi) = \eta(\varphi_a)$ for $\varphi \leq \varphi_a$, and $\eta(\varphi) = \eta(\varphi_b)$ for $\varphi \geq \varphi_b$. For $\varphi_a < \varphi < \varphi_b$ the function $\eta(\varphi)$ is affine linear, i.e. $\eta(\varphi) = \frac{1}{2}\left((\eta_2 - \eta_1)\varphi + (\eta_1 + \eta_2)\right)$.

We define $\overline{\rho} > \underline{\rho} > 0$, $\overline{\eta} \geq \underline{\eta} > 0$ fulfilling
- $\overline{\rho} \geq \rho(\varphi) \geq \underline{\rho} > 0$,
- $\overline{\eta} \geq \eta(\varphi) \geq \underline{\eta} > 0$,

see Remark 2.2.

(A5) The mean value of φ is zero, i.e. there holds $\frac{1}{|\Omega|}\int_\Omega \varphi \, dx = 0$. This can be achieved by choosing the values indicating the pure phases accordingly and considering a shifted system if required. In this case the values ± 1 change to some other appropriate values.

Remark 2.1. The Assumptions (A1)–(A3) are for example fulfilled by the polynomial free energy density

$$W^{poly}(\varphi) = \frac{1}{4}\left(1 - \varphi^2\right)^2.$$

Another free energy density fulfilling these assumptions is the relaxed double-obstacle free energy density given by

$$\begin{aligned}
\lambda(y) &:= \max(0, y-1) + \min(0, y+1), \\
\xi &:= \frac{1 + 2s + \sqrt{4s+1}}{2s}, \\
\delta &:= \frac{1}{2}\left(1 - \xi^2\right) + \frac{s}{3}|\lambda(\xi)|^3, \\
W^s(y) &= \frac{1}{2}\left(1 - (\xi y)^2\right) + \frac{s}{3}|\lambda(\xi y)|^3 + \delta
\end{aligned} \tag{9}$$

where $s > 0$, and as s denotes a penalisation parameter from Moreau–Yosida regularization s is chosen very large in practice. The energy density W^s can be understood as a relaxation of the double-obstacle free energy density

$$W^\infty(\varphi) = \begin{cases} \frac{1}{2}\left(1-\varphi^2\right) & \text{if } |\varphi| \leq 1, \\ \infty & \text{else,} \end{cases}$$

which is proposed in [16,49] to model phase separation. We note that here we use a cubic penalisiation to obtain the required regularity from (A1) and that ξ is chosen such that W^s takes its minima at ± 1 and δ is such that $W^s(\pm 1) = 0$. Let us note that the larger s, the better W^s reflects W^∞.

In the numerical examples of this work we use the free energy density $W \equiv W^s$. For this choice the splitting into convex and concave part reads

$$W_+(\varphi) = s\frac{1}{3}|\lambda(\xi\varphi)|^3, \qquad\qquad W_-(\varphi) = \frac{1}{2}(1-(\xi\varphi)^2) + \delta.$$

Furthermore we have

$$W_+'(\varphi) = s\xi|\lambda(\xi\varphi)|\lambda(\xi\varphi), \quad W_+''(\varphi) = 2s\xi^2|\lambda(\xi\varphi)|.$$

Remark 2.2. For the weak formulation of (1)–(8) we later require affine linearity of ρ on the image of φ. The affine linearity of η is assumed for simplicity. Note that in view of Assumption (A4), this essentially implies a bound on φ, namely $\varphi \in (\varphi_a, \varphi_b)$ as stated in Assumption (A4).

Using W^s as free energy density we argue, that for s sufficiently large (see [23, Rem. 6]) $|\varphi| \leq 1 + \theta$ holds, with θ sufficiently small, and in [45] it is shown for the Cahn–Hilliard equation without transport, that for the energy (9) in fact $\|\varphi\|_{L^\infty(\Omega)} \leq 1 + Cs^{-1/2}$ holds.

In a general setting one might use a nonlinear dependence between φ and ρ, see e.g. [2], or choose a cut-off procedure as proposed in [26, 29].

Anyway, since we later require linearity of ρ on the image of φ we state Assumption (A4) and note that this assumption is fulfilled in our numerical examples in Section 6.

Notation

We use the conventional notation for Sobolev and Hilbert Spaces, see e.g. [6]. With $L^p(\Omega)$, $1 \leq p \leq \infty$, we denote the space of measurable functions on Ω, whose modulus to the power p is Lebesgue-integrable. $L^\infty(\Omega)$ denotes the space of measurable functions on Ω, which are essentially bounded. For $p = 2$ we denote by $L^2(\Omega)$ the space of square integrable functions on Ω with inner product $(\cdot,\cdot)$ and norm $\|\cdot\|$. By $W^{k,p}(\Omega)$, $k \geq 1, 1 \leq p \leq \infty$, we denote the Sobolev space of functions admitting weak derivatives up to order k in $L^p(\Omega)$. If $p = 2$ we write $H^k(\Omega)$.

For $f \in H^1(\Omega)^n$ we introduce the continuous trace operator $\gamma : H^1(\Omega)^n \to H^{\frac{1}{2}}(\partial\Omega)^n$ as $\gamma f := f|_{\partial\Omega}$. Vice versa, for $g \in H^{\frac{1}{2}}(\partial\Omega)^n$ with $g \cdot \nu_\Omega = 0$ there exists $\widetilde{g} \in H^1(\Omega)^n$, $(\text{div}(\widetilde{g}), q) = 0\,\forall q \in L^2(\Omega)$ with $\gamma\widetilde{g} = g$ and $\|\widetilde{g}\|_{H^1(\Omega)^n} \leq C\|g\|_{H^{\frac{1}{2}}(\partial\Omega)^n}$, where C is independent of g, see [25, I. §2 Lem. 2.2]. We call $\widetilde{\cdot}$ the extension operator.

The subspace $H_0^1(\Omega)^n \subset H^1(\Omega)^n$ denotes the set of functions with vanishing boundary trace. We further set

$$L^2_{(0)}(\Omega) = \{v \in L^2(\Omega) \,|\, (v, 1) = 0\},$$

and with

$$H_\sigma(\Omega) = \{v \in H^1(\Omega)^n \,|\, (\text{div}(v), q) = 0\,\forall q \in L^2(\Omega)\}$$

we denote the space of all weakly solenoidal $H^1(\Omega)$ vector fields, i.e. we include the solenoidality condition in the distributional sense. We stress that there is no correspondence between the subscript σ and the scaled surface tension. We denote both terms using σ since these are standard notations. We further introduce

$$H_{0,\sigma}(\Omega) = H_0^1(\Omega)^n \cap H_\sigma(\Omega).$$

For $u \in L^q(\Omega)^n$, $q > 2$ if $n = 2$, $q \geq 3$ if $n = 3$, and $v, w \in H^1(\Omega)^n$ we introduce the trilinear form

$$a(u, v, w) = \frac{1}{2}\int_\Omega ((u\cdot\nabla)\, v)\, w\, dx - \frac{1}{2}\int_\Omega ((u\cdot\nabla)\, w)\, v\, dx. \tag{10}$$

Note that there holds $a(u, v, w) = -a(u, w, v)$, and especially $a(u, v, v) = 0$. We have the following stability estimate by Hölder inequalities and Sobolev embedding

$$|a(u, v, w)| \leq C\|u\|_{L^q(\Omega)}\|v\|_{H^1(\Omega)}\|w\|_{H^1(\Omega)}.$$

For a square summable series of functions $(f_m)_{m=1}^M \in V^M$, where $(V, \|\cdot\|_V)$ is a normed vector space, we introduce the notation $\|(f^m)_{m=1}^M\|_V^2 = \sum_{m=1}^M \|f_m\|_V^2$.

Finally for $v \in L^2(\Omega)^n, \varphi \in H^1(\Omega), \phi \in L^2(\Omega)$ we introduce the total energy $E(v, \varphi, \phi)$

$$E(v, \varphi, \phi) := \frac{1}{2}\int_\Omega \rho(\phi)|v|^2\, dx + \sigma\int_\Omega \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{\epsilon}W(\varphi)\, dx, \tag{11}$$

where the first integral is the kinetic energy and the second integral represents the Ginzburg–Landau energy of the phase field.

3. The time-discrete setting

In [23] existence of time discrete weak solutions for (1)–(4) is shown for the case of $g = 0$ and $f = 0$. In this section we formulate a time discrete optimization problem for (1)–(4), where we use g, f, and φ_0 as controls, and show existence of solutions together with first order optimality conditions.

Let $0 = t_0 < t_1 < \ldots < t_{m-1} < t_m < t_{m+1} < \ldots < t_M = T$ denote an equidistant subdivision of the interval $\overline{I} = [0, T]$ with $\tau_{m+1} - \tau_m \equiv \tau$ and sub intervals $I_0 = \{0\}$, $I_m = (t_{m-1}, t_m]$, $m = 1, \ldots, M$. From here onwards the superscript m denotes the corresponding variables at time instance t_m, e.g. $\varphi^m := \varphi(t_m)$. For functions $f \in L^2(0, T, V)$ we introduce $f^m := \fint_{I_m} f(t)\, dt \in V$. Note that this can be seen as a discontinuous Galerkin approximation using piecewise constant values.

We now introduce the optimal control problem under consideration. For this purpose we interpret φ_0, f, and g as sought control that we intend to choose, such that the corresponding phase field φ^M is close to a desired phase field φ_d in the mean square sense. If φ_d is the measurement of a real world system, then finding φ_0 such that the corresponding phase field φ^M is close to φ_d resembles an inverse problem.

We denote by $u \in U$ the control, where

$$U = U_I \times U_V \times U_B = \mathcal{K} \times L^2(0, T; \mathbb{R}^{u_v}) \times L^2(0, T; \mathbb{R}^{u_b})$$

is the space of controls, where

$$\mathcal{K} := \{v \in H^1(\Omega) \mid \int_\Omega v\, dx = 0, |v| \leq 1\} \subset H^1(\Omega) \cap L^\infty(\Omega)$$

denotes the space of admissible initial phase fields.

By

$$\mathcal{B}: U \to H^1(\Omega) \cap L^\infty(\Omega) \times L^2(0,T;L^2(\Omega)^n) \times L^2(0,T;(H^{1/2}(\partial\Omega))^n)$$

we denote the linear and bounded control operator, which consists of three components, i.e. $\mathcal{B} = [B_I, B_V, B_B]$, where $B_I(u_I,u_V,u_B) \equiv B_I u_I := u_I$, which is the initial phase field for the system, $B_V(u_I,u_V,u_B) \equiv B_V u_V$ with $B_V u_V(t,x) = \sum_{l=1}^{u_v} f_l(x) u_V^l(t)$ where $f_l \in L^2(\Omega)^n$ are given functions, which is a volume force acting on the fluid inside Ω, and $B_B(u_I,u_V,u_B) \equiv B_B u_B$, with $B_B u_B(t,x) = \sum_{l=1}^{u_b} g_l(x) u_B^l(t)$ where $g_l \in H^{1/2}(\partial\Omega)^n$ denote given functions, and this is a boundary force acting on the fluid as Dirichlet boundary data. To obtain a solenoidal velocity field, $B_B u_B$ has to fulfill the compatibility condition $\int_{\partial\Omega} B_B u_B \cdot \nu_\Omega \, ds = 0$, and in the following for simplicity we assume $g_l \cdot \nu_\Omega = 0$, $l = 1,\dots,u_b$, point wise.

Given a triple $(\alpha_I, \alpha_V, \alpha_B)$ of non negative values with $\alpha_I + \alpha_V + \alpha_B = 1$ we introduce an inner product for $u = (u_I,u_V,u_B) \in U$ and $v = (v_I,v_V,v_B) \in U$ by

$$(u,v)_U = \alpha_I (\nabla u_I, \nabla v_I)_{L^2(\Omega)} + \alpha_V (u_V,v_V)_{L^2(0,T;\mathbb{R}^{u_v})} + \alpha_B (u_B,v_B)_{L^2(0,T;\mathbb{R}^{u_b})} \tag{12}$$

and the norm $\|u\|_U^2 = (u,u)_U$.

We use the convention, that $\alpha_\star = 0$, $\star \in \{I,V,B\}$, means, that we do not apply this kind of control. If $\alpha_I = 0$ we use φ^0 as given data, if $\alpha_B = 0$, we assume no-slip boundary data for v. For notational convenience, in the following we assume $\alpha_\star \neq 0$ for all $\star \in \{I,V,B\}$.

We stress, that we do not discretize the control in time, although the state equation is time discrete. Thus we follow the concept of variational discretization [38]. Anyway, the control is discretized implicitly in time by the adjoint equation that we will derive later. We also note, that in view of the state equation, this allows us to dynamically adapt the time step size τ to the flow condition without changing the control space.

Following [23] we propose the following time discrete counterpart of (1)–(8):
Let $u \in U$ and $v_0 \in H_\sigma(\Omega) \cap L^\infty(\Omega)$ be given.

Initialization for $m = 1$:
Set $\varphi^0 = u_I$ and $v^0 = v_0$.
Find $\varphi^1 \in H^1(\Omega) \cap L^\infty(\Omega)$, $\mu^1 \in W^{1,3}(\Omega)$, $v^1 \in H_\sigma(\Omega)$, with $\gamma(v^1) = B_B u_B^1$, such that for all $w \in H_{0,\sigma}(\Omega)$, $\Phi \in H^1(\Omega)$, and $\Psi \in H^1(\Omega)$ it holds

$$\frac{1}{\tau}\int_\Omega \left(\frac{1}{2}(\rho^1+\rho^0)v^1 - \rho^0 v^0\right) w \, dx + a(\rho^1 v^0 + j^1, v^1, w)$$
$$+ \int_\Omega 2\eta^1 Dv^1 : Dw \, dx - \int_\Omega \mu^1 \nabla\varphi^0 w + \rho^0 K w \, dx - \left\langle B_V u_V^1, w \right\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} = 0, \tag{13}$$
$$\frac{1}{\tau}\int_\Omega (\varphi^1 - \varphi^0)\Psi \, dx + \int_\Omega (v^0 \cdot \nabla\varphi^0)\Psi \, dx + \int_\Omega b\nabla\mu^1 \cdot \nabla\Psi \, dx = 0, \tag{14}$$
$$\sigma\epsilon \int_\Omega \nabla\varphi^1 \cdot \nabla\Phi \, dx - \int_\Omega \mu^1 \Phi \, dx + \frac{\sigma}{\epsilon}\int_\Omega (W_+'(\varphi^1) + W_-'(\varphi^0))\Phi \, dx = 0, \tag{15}$$

where $j^1 := -\rho_\delta b \nabla\mu^1$.

Two-step scheme for $m > 1$:
Given $\varphi^{m-2} \in H^1(\Omega) \cap L^\infty(\Omega)$, $\varphi^{m-1} \in H^1(\Omega) \cap L^\infty(\Omega)$, $\mu^{m-1} \in W^{1,3}(\Omega)$, $v^{m-1} \in H_\sigma(\Omega)$,
find $v^m \in H_\sigma(\Omega)$, $\gamma(v^m) = B_B u_B^m$, $\varphi^m \in H^1(\Omega) \cap L^\infty(\Omega)$, $\mu^m \in W^{1,3}(\Omega)$ such that for all $w \in H_{0,\sigma}(\Omega)$, $\Psi \in H^1(\Omega)$,

and $\Phi \in H^1(\Omega)$ it holds

$$\frac{1}{\tau}\int_\Omega \left(\frac{\rho^{m-1}+\rho^{m-2}}{2}v^m - \rho^{m-2}v^{m-1}\right) w\,dx + \int_\Omega 2\eta^{m-1}Dv^m : Dw\,dx$$
$$+a(\rho^{m-1}v^{m-1}+j^{m-1},v^m,w)$$
$$-\int_\Omega \mu^m\nabla\varphi^{m-1}w + \rho^{m-1}Kw\,dx - \langle B_V u_V^m, w\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} = 0, \tag{16}$$
$$\int_\Omega \frac{\varphi^m-\varphi^{m-1}}{\tau}\Psi\,dx + \int_\Omega (v^m\cdot\nabla\varphi^{m-1})\Psi\,dx + \int_\Omega b\nabla\mu^m\cdot\nabla\Psi\,dx = 0, \tag{17}$$
$$\sigma\epsilon\int_\Omega \nabla\varphi^m\cdot\nabla\Phi\,dx - \int_\Omega \mu^m\Phi\,dx + \frac{\sigma}{\epsilon}\int_\Omega (W_+'(\varphi^m)+W_-'(\varphi^{m-1}))\Phi\,dx = 0, \tag{18}$$

where $j^{m-1} := -\rho_\delta b\nabla\mu^{m-1}$. We further use the abbreviations $\rho^m := \rho(\varphi^m)$ and $\eta^m := \eta(\varphi^m)$.

We note that in (16)–(18) the only nonlinearity arises from W_+' and thus only the equation (18) is nonlinear. A similar argumentation holds for (13)–(15). The regularity $\nabla\mu^{m-1}\in L^3(\Omega)$ is required for the trilinear form $a(\cdot,\cdot,\cdot)$, see (10).

Remark 3.1. We note that (16)–(18) is a two-step scheme for the phase field variable φ, and thus we need an initialization as proposed in (13)–(15). Here, as in [23] the sequential coupling of (14)–(15) and (13) is used as proposed in [46].

Another variant might be to require initial data on time instance t_{-1} for the phase field and at t_0 for the velocity field. Equations (17)–(18) can than be solved for φ^0 and μ^0 to obtain initial values, see [34].

Since we are later also interested in control of the initial value φ_0 we propose the initialization scheme (13)–(15) here.

Remark 3.2. For the rest of this paper we discuss optimal control of the time discrete system (13)–(18) for a fixed parameter τ. We neither discuss the dependence of our results with respect to the limit $\tau\to 0$, nor with respect to the limit $\epsilon\to 0$. In the subsequent analysis constants depend critically on ϵ as e.g. powers of ϵ^{-1} result from estimates involving Young's inequality.

We refer to [26] for investigations related to the case $\tau\to 0$, and to [19, 21] for investigations considering the case $\epsilon\to 0$ for the Allen–Cahn system.

Theorem 3.3. *Let $v^0\in H_\sigma(\Omega)\cap L^\infty(\Omega)^n$ and $u\in U$ be given data.*

Then there exists a unique solution (v^1,φ^1,μ^1) to (13)–(15), and it holds

$$\|v^1\|_{H^1(\Omega)^n} + \|\varphi^1\|_{H^2(\Omega)} + \|\mu^1\|_{H^2(\Omega)}$$
$$\le C_1(v_0)C_2\left(\|u_I\|_{H^1(\Omega)}, \|B_V u_V^1\|_{L^2(\Omega)^n}, \|B_B u_B^1\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right) \tag{19}$$

and φ^1,μ^1 can be found by Newton's method. The constants C_1, C_2 depend polynomially on its arguments, on the system parameter and especially ϵ^{-1}.

Proof. The existence of $(\varphi^1,\mu^1)\in H^1(\Omega)\times H^1(\Omega)$ follows from [33]. There the corresponding system without the transport term $v^0\nabla u_I$ is analyzed. This term is a given volume force, that can be incorporated in a straightforward manner. From this we directly obtain the stability inequality

$$\|\varphi^1\|_{H^1(\Omega)} + \|\mu^1\|_{H^1(\Omega)} \le C_1(v^0)C_2(\|u_I\|_{H^1(\Omega)}).$$

Since $|W_+'(\varphi)|\le C(1+|\varphi|^q|)$, $q\le 3$ we have $W_+'(\varphi)\in L^2(\Omega)$ and by L^2 regularity theory we have $\varphi^1\in H^2(\Omega)$ and

$$\|\varphi^1\|_{H^2(\Omega)} \le C(\|\mu^1\|_{H^1(\Omega)}, \|\varphi^1\|_{H^1(\Omega)}, \|u_I\|_{H^1(\Omega)}).$$

We further have $v^0 \nabla u_I \in L^2(\Omega)$ and thus we have $\mu^1 \in H^2(\Omega)$ and the stability inequality

$$\|\mu^1\|_{H^2(\Omega)} \le C_1(v_0) C_2(\|u_I\|_{H^1(\Omega)}, \|\varphi^1\|_{H^1(\Omega)}).$$

Convergence of Newton's method directly follows from [33]. Note that the only nonlinearity W_+' is monotone.

With v^0, φ^1, u_I, and μ^1 given data, (13) defines a coercive and continuous bilinear form on H_σ and thus existence and stability of a solution follows from Lax-Milgram's theorem. This uses the antisymmetry of the trilinear form a and Korn's inequality. The non-homogeneous Dirichlet data are incorporated by extension. Note that (13) is linear with respect to v^1, and also compare the proof of Theorem 3.4. □

Theorem 3.4. *Let $v^{m-1} \in H_\sigma(\Omega)$, $\varphi^{m-2} \in H^1(\Omega) \cap L^\infty(\Omega)$, $\varphi^{m-1} \in H^1(\Omega) \cap L^\infty(\Omega)$, and $\mu^{m-1} \in W^{1,3}(\Omega)$, be given data. Then there exists a unique solution (v^m, φ^m, μ^m) to (16)–(18).*

It further holds $\varphi^m \in H^2(\Omega)$ and if additionally $\varphi^{m-1} \in W^{1,3}(\Omega)$ we have $\mu^m \in H^2(\Omega)$ and the stability inequality

$$\begin{aligned}\|v^m\|_{H^1(\Omega)^n} + &\|\mu^m\|_{H^2(\Omega)} + \|\varphi^m\|_{H^2(\Omega)} \\ &\le C\left(\|v^{m-1}\|_{H^1(\Omega)^n}, \|\varphi^{m-1}\|_{W^{1,3}(\Omega)}, \|B_V u_V^m\|_{L^2(\Omega)^n}, \|B_B u_B^m\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right),\end{aligned}$$

holds. The constant C depends polynomially on its arguments, on the system parameter and especially ϵ^{-1}. Locally the unique solution can be found by Newton's method.

Proof. In [23] the existence for $\gamma(B_B u_B^m) = 0$ and $B_V u_V^m = 0$ is shown using a Galerkin approach. The additional volume force is incorporated in a straight forward manner. The boundary data $B_B u_B^m$ is introduced by investigating a shifted system, i.e. by considering $v^m = v_0^m + \widetilde{B_B u_B^m}$, where v_0^m has zero Dirichlet data. Note that due to the linearity of (16) with respect to v^m the terms involving $\widetilde{B_B u_B^m}$ are independent of the solution on the current time instance, and also appear as volume force.

To derive the stability estimate, we proceed as follows. We define $e := \widetilde{B_B u_B^m}$, i.e. a solenoidal extension of $B_B u_B^m$ into Ω, and use $w = v^m - e$ as test function in (16), $\Psi = \mu^m$ as test function in (17), and $\Phi = \tau^{-1}(\varphi^m - \varphi^{m-1})$ as test function in (18), and add the resulting equations. Using the properties of W_+' and W_-' we obtain (compare [23, Thm. 7])

$$\begin{aligned}&E(v^m, \varphi^m, \varphi^{m-1}) + \frac{1}{2}\int_\Omega \rho^{m-2}|v^m - v^{m-1}|^2\,dx + 2\tau\int_\Omega \eta^{m-1}|Dv^m|^2\,dx \\ &+ \tau\int_\Omega b|\nabla\mu^m|^2\,dx + \frac{\sigma\epsilon}{2}\|\nabla\varphi^m - \nabla\varphi^{m-1}\|^2 \\ &\le E(v^{m-1}, \varphi^{m-1}, \varphi^{m-2}) + \int_\Omega\left(\frac{\rho^{m-1} + \rho^{m-2}}{2}v^m - \rho^{m-2}v^{m-1}\right)e\,dx \\ &+ \tau a(\rho^{m-1}v^{m-1} + J^{m-1}, v^m, e) + 2\tau\int_\Omega \eta^{m-1}Dv^m : De\,dx \\ &- \tau\int_\Omega \mu^m\nabla\varphi^{m-1}e\,dx + (\rho^{m-1}K, v^m - e) + \tau(B_V u_V^m, v^m - e)_{L^2(\Omega)^n}.\end{aligned} \tag{20}$$

Note that for $e \equiv 0$, i.e. $v^m|_{\partial\Omega} \equiv 0$, this result is shown in [23, Thm. 7]. For the left hand side of the inequality (20) we have using (A4), (A5)

$$\frac{1}{2}\underline{\rho}\|v^m\|^2 + \frac{\sigma\epsilon}{2(1 + C_p^2)}\|\varphi^m\|_{H^1(\Omega)}^2 \le E(v^m, \varphi^m, \varphi^{m-1}), \quad 2\tau\underline{\eta}\|Dv^m\|^2 \le 2\tau\int_\Omega \eta^{m-1}|Dv^m|^2\,dx,$$

where C_p denotes the constant from Poincaré's inequality. Thus for the left hand side we have by Korn's inequality, i.e. $\|v\|^2_{H^1(\Omega)^n} \leq C(\|v\|^2 + \|Dv\|^2)$, the lower bound

$$C\left(\|v^m\|^2_{H^1(\Omega)^n} + \|\varphi^m\|^2_{H^1(\Omega)} + \|\nabla\mu^m\|^2\right).$$

Next we observe since $e|_{\partial\Omega} = g$ and $g \cdot \nu_\Omega = 0$ that for any $\beta \in \mathbb{R}$ it holds

$$\int_\Omega \beta\nabla\varphi^{m-1} e\,dx = -\int_\Omega \operatorname{div}(\beta e)\varphi^{m-1}\,dx + \int_{\partial\Omega} e\cdot\nu_\Omega\varphi^{m-1}\,ds = 0, \tag{21}$$

and thus $\int_\Omega \mu^m\nabla\varphi^{m-1}e\,dx = \int_\Omega(\mu^m - \int_\Omega\mu^m)\nabla\varphi^{m-1}e\,dx$ holds.

For the right hand side we have

$$\begin{aligned}
E(v^{m-1},\varphi^{m-1},\varphi^{m-2}) &\leq C\left(\|v^{m-1}\|^2 + \|\nabla\varphi^{m-1}\|^2 + 1 + \|\varphi^{m-1}\|^4_{L^4(\Omega)}\right),\\
\int_\Omega\left(\frac{\rho^{m-1}+\rho^{m-2}}{2}v^m - \rho^{m-2}v^{m-1}\right)e\,dx &\leq C\left(\|v^m\| + \|v^{m-1}\|\right)\|e\|,\\
\tau a(\rho^{m-1}v^{m-1} + J^{m-1}, v^m, e) &\leq C\|\rho^{m-1}v^{m-1} + J^{m-1}\|_{L^3(\Omega)}\|v^m\|_{H^1(\Omega)^n}\|e\|_{H^1(\Omega)^n},\\
2\tau\int_\Omega \eta^{m-1}Dv^m : De\,dx &\leq C\|\nabla v^m\|\|\nabla e\|,\\
\tau\int_\Omega \mu^m\nabla\varphi^{m-1}e\,dx &\leq C\|\mu^m - \int_\Omega\mu^m\,dx\|_{L^4(\Omega)}\|\nabla\varphi^{m-1}\|\|e\|_{L^4(\Omega)} \leq C\|\nabla\mu^m\|\|\varphi^{m-1}\|_{H^1(\Omega}\|e\|_{H^1(\Omega)^n},\\
(\rho^{m-1}K, v^m - e) &\leq \overline{\rho}|K|\|v^m\|_{L^2(\Omega)^n},\\
\tau(B_V u_V^m, v^m - e)_{L^2(\Omega)^n} &\leq \|B_V u_V^m\|\|v^m\| + \|B_V u_V^m\|\|e\|.
\end{aligned}$$

The bound for $\|v^m\|_{H^1(\Omega)^n}$, $\|\varphi^m\|_{H^1(\Omega)}$ and $\|\nabla\mu^m\|$ now follows from a3 scaled Young's inequality and compensating the terms involving μ^m and v^m on the left hand side.

To bound $\|\mu^m\|$ it is sufficient to bound $\int_\Omega\mu^m\,dx$ and to use Poincaré's inequality. The required bound is obtained by testing (18) with $\Phi \equiv 1$, using (A3) and the already shown bound on φ^m.

The local convergence of Newton's method is shown in [23].

The regularity $\varphi^m, \mu^m \in H^2(\Omega)$ follow as in the proof of Theorem 3.3, but now using $\nabla\varphi^{m-1} \in L^3(\Omega)$ and $v^m \in H_\sigma \hookrightarrow L^6(\Omega)$.

□

Let us next introduce the optimization problem under investigation. For this we first rewrite (13)–(18) in a compact and abstract form and introduce

$$\begin{aligned}
Y &:= H_\sigma(\Omega)^M \times \left(H^1(\Omega)\cap L^\infty(\Omega)\right)^M \times W^{1,3}(\Omega)^M,\\
Y_0 &:= H_{0,\sigma}(\Omega)^M \times \left(H^1(\Omega)\cap L^\infty(\Omega)\right)^M \times W^{1,3}(\Omega)^M,\\
y &:= (v^m,\varphi^m,\mu^m)_{m=1}^M \in Y,\\
Z &:= \left(H_{0,\sigma}(\Omega)^M \times H^1(\Omega)^M \times H^1(\Omega)^M\right)^\star,
\end{aligned}$$

$$\begin{aligned}
e : Y_0 \times U &\to Z,\\
e(y_0, u) &= 0.
\end{aligned} \tag{22}$$

The operator e is defined as follows

$$
\begin{aligned}
&\langle \tilde y, e(y_0,u)\rangle_{Z^\star,Z} :=\\
&\tau^{-1}\left(\frac{1}{2}(\rho^1+\rho^0)(v_0^1+\widetilde{B_Bu_B^1})-\rho^0v^0,\tilde v^1\right)+a(\rho^1v^0+j^1,v_0^1+\widetilde{B_Bu_B^1},\tilde v^1)\\
&+(2\eta^1D(v_0^1+\widetilde{B_Bu_B^1}),D\tilde v^1)-(\mu^1\nabla u_1+\rho^0K,\tilde v^1)\\
&-(B_Vu_V^1,\tilde v^1)\\
&+\tau^{-1}(\varphi^1-u_1,\tilde\varphi^1)+(v^0\nabla u_1,\tilde\varphi^1)+(b\nabla\mu^1,\nabla\tilde\varphi^1)\\
&+\sigma\epsilon(\nabla\varphi^1,\nabla\tilde\mu^1)-(\mu^1,\tilde\mu^1)\\
&+\sigma\epsilon^{-1}(W_+'(\varphi^1)+W_-'(u_I),\tilde\mu^1)\\
+\sum_{m=2}^M&\Bigg[\tau^{-1}\left(\frac{1}{2}(\rho^{m-1}+\rho^{m-2})(v_0^m+\widetilde{B_Bu_B^m})-\rho^{m-2}(v_0^{m-1}+\widetilde{B_Bu_B^{m-1}}),\tilde v^m\right)\\
&+a(\rho^{m-1}(v_0^{m-1}+\widetilde{B_Bu_B^{m-1}})+j^{m-1},v_0^m+\widetilde{B_Bu_B^m},\tilde v^m)\\
&+(2\eta^{m-1}D(v_0^m+\widetilde{B_Bu_B^m}),D\tilde v^m)-(\mu^m\nabla\varphi^{m-1}+\rho^{m-1}K,\tilde v^m)\\
&-(B_Vu_V^m,\tilde v^m)\\
&+\tau^{-1}(\varphi^m-\varphi^{m-1},\tilde\varphi^m)+((v_0^m+\widetilde{B_Bu_B^m})\nabla\varphi^{m-1},\tilde\varphi^m)+(b\nabla\mu^m,\nabla\tilde\varphi^m)\\
&+\sigma\epsilon(\nabla\varphi^m,\nabla\tilde\mu^m)-(\mu^m,\tilde\mu^m)\\
&+\sigma\epsilon^{-1}(W_+'(\varphi^m)+W_-'(\varphi^{m-1}),\tilde\mu^m)\Bigg]
\end{aligned}
$$

with $y_0 := (v_0^m,\varphi^m,\mu^m)_{m=1}^M \in Y_0$, and $\tilde y = ((\tilde v^m)_{m=1}^M,(\tilde\varphi^m)_{m=1}^M,(\tilde\mu^m)_{m=1}^M)))) \in Z^\star$. Here again $\rho^m := \rho(\varphi^m)$, $\eta^m := \eta(\varphi^m)$ and especially $\rho^0 := \rho(u_I)$, $\eta^0 := \eta(u_I)$.

Now the time-discrete optimization problem under investigation is given as

$$
\begin{aligned}
\min_{u\in U} J((\varphi^m)_{m=1}^M,u) = &\frac{1}{2}\|\varphi^M-\varphi_d\|^2_{L^2(\Omega)}\\
&+\frac{\alpha}{2}\left(\alpha_I\int_\Omega\frac{\epsilon}{2}|\nabla u_I|^2+\epsilon^{-1}W_u(u_I)\,dx\right.\\
&\left.+\alpha_V\|u_V\|^2_{L^2(0,T;\mathbb{R}^{u_v})}+\alpha_B\|u_B\|^2_{L^2(0,T;\mathbb{R}^{u_b})}\right)\\
s.t.\ e(y,u)=0.&
\end{aligned}
\tag{$\mathcal{P}$}
$$

Here $\varphi_d \in L^2(\Omega)$ is a given desired phase field, and $\alpha > 0$ is a weight for the control cost. For the control cost of the initial value we use the well-known Ginzburg–Landau energy (11) of the phase field u_I with interfacial thickness ϵ. Here we use the double obstacle free energy density $W_u \equiv W^\infty$ given in Remark 2.1. In our numerical examples it is advantageous to use this non-smooth free energy density instead of the smoother one used in the Cahn-Hilliard/Navier-Stokes system for the simulation.

Theorem 3.5. *Let $v^0 \in H_\sigma(\Omega)\cap L^\infty(\Omega)$, $u\in U$ be given.*

Then there exists a unique solution to the equation $e(y,u) = 0$*, i.e. there exist* $(v^m, \varphi^m, \mu^m)_{m=1}^M \in Y$ *such that* (v^m, φ^m, μ^m) *is the unique solution to* (13)–(18) *for* $m = 1, \dots, M$*. Moreover there holds*

$$\|(v^m)_{m=1}^M\|_{H^1(\Omega)^n} + \|(\varphi^m)_{m=1}^M\|_{H^2(\Omega)} + \|(\mu^m)_{m=1}^M\|_{H^2(\Omega)} \\ \leq C_1\left(v^0\right) C_2\left(\|u_I\|_{H^1(\Omega)}, \|(B_V u_V^m)_{m=1}^M\|_{L^2(\Omega)^n}, \|(B_B u_B^m)_{m=1}^M\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right).$$

Further $e(y,u)$ *is Fréchet-differentiable with respect to* y*, and* $e_y(y,u) \in \mathcal{L}(Y_0, Z)$ *has a bounded inverse. Thus Newton's method can be applied for finding the unique solution of* (22) *for given* u*.*

Proof. The existence and stability of the solution for each time instance follows directly from Theorem 3.3 and Theorem 3.4.

The equation $e(y,u) = 0$ is of block diagonal form with nonlinear entries on the diagonal. Thus solving (22) reduces to solving each time instance with given data from the previous time instance. As argued in Theorem 3.3 and Theorem 3.4 these nonlinear equations can be solved by Newton's method. Applying this argument for all time instances we obtain that $e_y(y,u) \in \mathcal{L}(Y_0, Z)$ has a bounded inverse. □

Lemma 3.6. *The functional* $J(y_0, u)$ *is continuously differentiable with respect to* y_0 *and* u*.*

Based on Theorem 3.5 we introduce the reduced functional $\hat{J}(u) := J(y_0(u), u)$ and state the following theorem.

Theorem 3.7 (Existence of an optimal control)**.** *There exists at least one solution to* $\mathcal{P}$*, i.e. at least one optimal control.*

Proof. Since $\hat{J}$ is bounded from below, there exists a minimizing sequence u_l with $\hat{J}(u_l) \to \hat{J}^\star$ and $\hat{J}^\star := \inf_u \hat{J}(u)$.

Since $\hat{J}$ is radially unbounded, there exists $V \subset U$, bounded, convex and closed such that $u_l \subset V$ and thus there exists a weakly convergent subsequence, in the following again denoted by (u_l). Since closed convex sets are weakly closed, $u_l \rightharpoonup u_\star \in V$ holds. Let $y_l = (v_l, \varphi_l, \mu_l)$ denote the unique solution of (13)–(18) for u_l. Then $y_l \rightharpoonup y_\star \in Y$, with $y_\star = y_\star(u_\star)$, and $(u_\star, y_\star)$ solves (13)-(18). This can be shown as in [23, Thm. 6].

It remains to show, that $J(u_\star) = J^\star$. To begin with we note that $y_l \rightharpoonup y_\star$ holds, which implies $\varphi_l^M \rightharpoonup \varphi_\star^M$ in $H^1(\Omega)$ and $\varphi_l^M \to \varphi_\star^M$ in $L^2(\Omega)$ by Rellich's theorem. This gives convergence for the first addend in $(\mathcal{P})$. Concerning the second addend we note that again Rellich's theorem gives $u_{I_l} \to u_{I_\star} \in \mathcal{K}$ in $L^2(\Omega)$, and thus pointwise a.e. This gives $W_u(u_{I_l}) \to W_u((u_I)_\star)$ pointwise a.e.. The claim now follows from the weak lower semicontinuity of norms, which implies that

$$\hat{J}(u_\star) \leq \liminf \hat{J}(u_l) = \hat{J}^\star$$

holds. Thus $u_\star$ is an optimal control. □

We next derive first order optimality conditions in the abstract setting. We introduce an adjoint state $p \in Z^\star$ and the Lagrangian as

$$L(y,p,u) := J(y,u) - \langle p, e(y,u)\rangle_{Z^\star, Z}\,.$$

By Lagrangian calculus we then obtain the following first order optimality conditions.

Theorem 3.8 (First order optimality conditions in abstract setting)**.** *Let* $u \in U$*,* $y \in Y$ *be an optimal solution to* $\mathcal{P}$*. Then there exists an adjoint state* $p \in Z^\star$ *and the triple* (u, y, p) *fulfills the following first order optimality* *conditions:*

$$e(y,u) = 0 \in Z, \tag{23}$$
$$(e_y(y,u))^\star p = J_y(y,u) \in Y_0^\star, \tag{24}$$
$$\langle J_u(y,u) + (e_u(y,u))^\star p, w-u\rangle_{U^\star,U} = 0 \quad \forall w \in U. \tag{25}$$

Proof. From Theorem 3.5 and Lemma 3.6 we have that e and J fulfill the assumptions of [41, Cor. 1.3], which in turn asserts the claim. □

To state the first order optimality system we introduce Lagrange multiplier $p \in Z^\star$, $p = (p_v^m, p_\varphi^m, p_\mu^m)_{m=1}^M \in H_{0,\sigma}^M \times H^1(\Omega)^M \times H^1(\Omega)^M$ and define the Lagrangian

$$L : U \times (H_{0,\sigma})^M \times (H^1(\Omega)\cap L^\infty(\Omega))^M \times W^{1,3}(\Omega)^M$$
$$\times (H_{0,\sigma})^M \times H^1(\Omega)^M \times H^1(\Omega)^M \to \mathbb{R}$$

as

$$\begin{aligned}
&L(u, v_0^m, \varphi^m, \mu^m, p_v^m, p_\varphi^m, p_\mu^m) := \frac{1}{2}\|\varphi^M - \varphi_d\|^2_{L^2(\Omega)}\\
&+ \frac{\alpha}{2}\left(\alpha_V \|u_V\|^2_{L^2(0,T;\mathbb{R}^{u_v})} + \alpha_B\|u_B\|^2_{L^2(0,T;\mathbb{R}^{u_b})} + \alpha_I\left(\int_\Omega \frac{\delta}{2}|\nabla u_I|^2 + \frac{1}{\delta}W_u(u_I)\,dx\right)\right)\\
&- \sum_{m=2}^M \Bigg[\frac{1}{\tau}\left(\frac{\rho^{m-1}+\rho^{m-2}}{2}(v_0^m + \widetilde{B_B u_B^m}) - \rho^{m-2}(v_0^{m-1} + \widetilde{B_B u_B^{m-1}}), p_v^m\right)\\
&+ a(\rho^{m-1}(v_0^{m-1} + \widetilde{B_B u_B^{m-1}}) + j^{m-1}, (v_0^m + \widetilde{B_B u_B^m}), p_v^m)\\
&+ (2\eta^{m-1} D(v_0^m + \widetilde{B_B u_B^m}), Dp_v^m)\\
&-(\mu^m \nabla\varphi^{m-1}, p_v^m) - (\rho^{m-1}K, p_v^m) - (B_V u_V^m, p_v^m)\Bigg]\\
&- \sum_{m=2}^M \left[\frac{1}{\tau}(\varphi^m - \varphi^{m-1}, p_\varphi^m) + ((v_0^m + \widetilde{B_B u_B^m})\nabla\varphi^{m-1}, p_\varphi^m) + (b\nabla\mu^m, \nabla p_\varphi^m)\right]\\
&- \sum_{m=2}^M \left[\sigma\epsilon(\nabla\varphi^m, \nabla p_\mu^m) - (\mu^m, p_\mu^m) + \frac{\sigma}{\epsilon}\left(W'_+(\varphi^m) + W'_-(\varphi^{m-1}), p_\mu^m\right)\right]\\
&- \Bigg[\frac{1}{\tau}\left(\frac{\rho^1+\rho^0}{2}(v^1 + \widetilde{B_B u_B^1}) - \rho^0 v^0, p_v^1\right) + a(\rho^1 v^0 + j^1, (v^1 + \widetilde{B_B u_B^1}), p_v^1)\\
&+(2\eta^1 D(v^1 + \widetilde{B_B u_B^1}), Dp_v^1) - (\mu^1\nabla u_I, p_v^1) - (\rho^0 K, p_v^1) - (B_V u_V^1, p_v^1)\Bigg]\\
&- \left[\frac{1}{\tau}(\varphi^1 - u_I, p_\varphi^1) + (v^0\nabla u_I, p_\varphi^1) + (b\nabla\mu^1, \nabla p_\varphi^1)\right]\\
&- \left[\sigma\epsilon(\nabla\varphi^1, \nabla p_\mu^1) - (\mu^1, p_\mu^1) + \frac{\sigma}{\epsilon}\left(W'_+(\varphi^1) + W'_-(u_I), p_\mu^1\right)\right].
\end{aligned}$$

Here again $\rho^m := \rho(\varphi^m)$, $\eta^m := \eta(\varphi^m)$ and especially $\rho^0 := \rho(u_1)$, $\eta^0 := \eta(u_1)$. In the following we write $v^m := v_0^m + \widetilde{B_B u_B^m}$.

The optimality system is now given by $(DL(x), \tilde{x} - x) \geq 0$, where x abbreviates all arguments of L and $\tilde{x}$ denotes an admissible direction. For all components of x except u_I it even holds $(DL(x), \tilde{x}) = 0$ since there no further constraints apply, while U_I is a convex subset of $H^1(\Omega) \cap L^\infty(\Omega)$.

Derivative with respect to the velocity
The derivative with respect to v_0^m for $m = 2, \ldots, M$ into a direction $\tilde{v} \in H_{0,\sigma}$ is given by

$$
\begin{aligned}
(D_{v^m} L(\ldots, v^m, \ldots), \tilde{v}) = \\
&- \frac{1}{\tau}\left((\frac{\rho^{m-1} + \rho^{m-2}}{2}\tilde{v}, p_v^m) - (\rho^{m-1}\tilde{v}, p_v^{m+1}) \right) \\
&- a(\rho^m \tilde{v}, v_0^{m+1} + \widetilde{B_B u_B^{m+1}}, p_v^{m+1}) \\
&- a(\rho^{m-1}(v_0^{m-1} + \widetilde{B_B u_B^{m-1}}) + j^{m-1}, \tilde{v}, p_v^m) \\
&- (2\eta^{m-1} D\tilde{v}, Dp_v^m) - (\tilde{v}\nabla\varphi^{m-1}, p_\varphi^m) = 0.
\end{aligned}
\tag{26}
$$

For $m = 1$ we get

$$
\begin{aligned}
(D_{v^1} L(\ldots, v^1, \ldots), \tilde{v}) = \\
&\frac{1}{\tau}(\rho^0 \tilde{v}, p_v^2) - a(\rho^1 \tilde{v}, v_0^2 + \widetilde{B_B u_B^2}, p_v^2) \\
&- \frac{1}{2\tau}((\rho^1 + \rho^0)\tilde{v}, p_v^1) - a(\rho^1(v_0^0 + \widetilde{B_B u_B^0}) + j^1, \tilde{v}, p_v^1) - (2\eta^1 D\tilde{v}, Dp_v^1) = 0.
\end{aligned}
\tag{27}
$$

Note that for notational convenience here we introduce artificial variables v_0^{M+1}, p_v^{M+1}, u_B^{M+1} and set them to $v_0^{M+1} \equiv p_v^{M+1} \equiv 0$, $u_B^{M+1} = 0$.

Remark 3.9. Note that we derive the adjoint system in the solenoidal setting. Introducing a variable π for the pressure in the primal equation leads to an additional adjoint variable p_π for the adjoint pressure and to an additional term $(-div\tilde{v}, p_\pi)$.

Derivative with respect to the chemical potential
The derivative with respect to the chemical potential for $m = 2, \ldots, M$ in a direction $\tilde{\mu} \in W^{1,3}(\Omega)$ is

$$
\begin{aligned}
(D_{\mu^m} L(\ldots, \mu^m, \ldots), \tilde{\mu}) = \\
&- a(j_{\mu^m}^m \tilde{\mu}, v^{m+1}, p_v^{m+1}) + (\tilde{\mu}\nabla\varphi^{m-1}, p_v^m) - (b\nabla\tilde{\mu}, \nabla p_\varphi^m) + (\tilde{\mu}, p_\mu^m) = 0.
\end{aligned}
\tag{28}
$$

For $m = 1$ the equations is

$$
\begin{aligned}
(D_{\mu^1} L(\ldots, \mu^1, \ldots), \tilde{\mu}) = \\
&- a(j_\mu^1 \tilde{\mu}, v^2, p_v^2) - a(j_\mu^1 \tilde{\mu}, v^1, p_v^1) + (\tilde{\mu}\nabla u_I, p_v^1) - (b\nabla\tilde{\mu}, \nabla p_\varphi^1) + (\tilde{\mu}, p_\mu^1) = 0.
\end{aligned}
\tag{29}
$$

Here for $m = 1, \ldots, M$ we abbreviate $j_\mu^m \tilde{\mu} = -\rho_\delta b \nabla\tilde{\mu}$, and for notational convenience we introduce artificial variables $v^{M+1} = v_0^{M+1} + \widetilde{B_B u_B^{M+1}}$, p_v^{M+1}, and set them to $v^{M+1} \equiv p_v^{M+1} \equiv 0$.

The above also contains the boundary condition

$$
\nabla p_\varphi^m \cdot \nu_\Omega = 0 \quad m = 1, \ldots, M,
$$

in weak form, which for smooth p_φ^m follows from integration by parts.

Derivative with respect to the phase field
The derivative with respect to the phase field φ^m in a direction $\tilde{\varphi} \in H^1(\Omega) \cap L^\infty(\Omega)$ is for $m = 2, \dots, M$

$$
\begin{aligned}
&(D_{\varphi^m} L(\dots, \varphi^m, \dots), \tilde{\varphi}) = \\
&\quad \delta_{mM}(\varphi^m - \varphi_d, \tilde{\varphi}) - \frac{1}{\tau}\left(\rho' \frac{v^{m+1} p_v^{m+1} + v^{m+2} p_v^{m+2}}{2}, \tilde{\varphi}\right) + \frac{1}{\tau}\left(\rho' v^{m+1} p_v^{m+2}, \tilde{\varphi}\right) \\
&\quad - a(\rho' \tilde{\varphi} v^m, v^{m+1}, p_v^{m+1}) - (2\eta' \tilde{\varphi} D v^{m+1}, D p_v^{m+1}) \\
&\quad + (\mu^{m+1} \nabla \tilde{\varphi}, p_v^{m+1}) + (\rho' \tilde{\varphi} K, p_v^{m+1}) \\
&\quad - \frac{1}{\tau}\left((\tilde{\varphi}, p_\varphi^m) - (\tilde{\varphi}, p_\varphi^{m+1})\right) - (v^{m+1} \nabla \tilde{\varphi}, p_\varphi^{m+1}) \\
&\quad - \sigma\epsilon(\nabla\tilde{\varphi}, \nabla p_\mu^m) - \frac{\sigma}{\epsilon}(W_+''(\varphi^m)\tilde{\varphi}, p_\mu^m) - \frac{\sigma}{\epsilon}(W_-''(\varphi^m)\tilde{\varphi}, p_\mu^{m+1}) = 0,
\end{aligned}
\tag{30}
$$

where δ_{mM} denotes the Kronecker delta. For $m = 1$ we get

$$
\begin{aligned}
&(D_{\varphi^1} L(\dots, \varphi^1, \dots), \tilde{\varphi}) = \\
&\quad - \frac{1}{\tau}(\frac{\rho'}{2}\tilde{\varphi}, v^2 p_v^2) - a(\rho' \tilde{\varphi} v^1, v^2, p_v^2) - a(\rho' \tilde{\varphi} v^0, v^1, p_v^1) \\
&\quad - (2\eta' \tilde{\varphi} D v^2, D p_v^2) - (2\eta' \tilde{\varphi} D v^1, D p_v^1) - (\mu^2 \nabla \tilde{\varphi} p_v^2) - (\rho' \tilde{\varphi} K, p_v^2) \\
&\quad + \frac{1}{\tau}(\tilde{\varphi}, p_\varphi^2) - (v^2 \nabla \tilde{\varphi}, p_\varphi^2) - \frac{\sigma}{\epsilon}(W_-''(\varphi^1)\tilde{\varphi}, p_\mu^2) \\
&\quad - \frac{1}{\tau}(\frac{\rho' \tilde{\varphi}}{2} v^1, p_v^1) - \frac{1}{\tau}(\tilde{\varphi}, p_\varphi^1) - \sigma\epsilon(\nabla\tilde{\varphi}, \nabla p_\mu^1) - \frac{\sigma}{\epsilon}(W_+''(\varphi^1)\tilde{\varphi}, p_\mu^1) = 0.
\end{aligned}
\tag{31}
$$

Here for notational convenience we introduce artificial variables $v^{M+1} = v_0^{M+1} + \widetilde{B_B u_B^{M+1}}$, $v^{M+2} = v_0^{M+2} + \widetilde{B_B u_B^{M+2}}$, p_v^{M+1}, p_v^{M+2}, and set them to zero.

The above also contains the boundary condition

$$
\nabla p_\mu^m \cdot \nu_\Omega = 0 \quad m = 1, \dots, M,
$$

in weak form, which for smooth p_μ^m follows from integration by parts.

Derivative with respect to the control
Finally we calculate the derivative with respect to the control for the three parts of the control space.

For a test direction $w \in U_V$ we have

$$
(D_{u_V} L(u, \dots), w) = \alpha\alpha_V \int_I (u_V, w)_{\mathbb{R}^{u_v}}\, dt + \sum_{m=1}^{M} (B_V w^m, p_v^m)_{L^2(\Omega)} = 0,
$$

and thus the optimality condition is

$$
\alpha\tau\alpha_V u_V^m + B_V^\star p_v^m = 0 \in \mathbb{R}^{u_v} \quad m = 1, \dots, M \tag{32}
$$

Here $B_V^\star p_v^m$ is defined as

$$
B_V^\star p_v^m := ((f_l, p_v^m)_{L^2(\Omega)^n})_{l=1}^{u_v}.
$$

Concerning the derivative with respect to u_B we have for a test function $w \in U_B$

$$
\begin{aligned}
(D_{u_B} L(u,\ldots), w) = \alpha\alpha_B \int_I (u_B, w)_{\mathbb{R}^{u_b}}\,dt - \tau^{-1}\left(\frac{\rho^1+\rho^0}{2}\widetilde{B_B w^1}, p_v^1\right) \\
- a(\rho^1 v^0 + j^1, \widetilde{B_B w^1}, p_v^1) - 2(\eta^1 D\widetilde{B_B w^1}, Dp_v^1) \\
- \sum_{m=2}^{M}\Bigg[\tau^{-1}\left(\frac{\rho^{m-1}+\rho^{m-2}}{2}\widetilde{B_B w^m}, p_v^m\right) - \left(\rho^{m-2}\widetilde{B_B w^{m-1}}, p_v^m\right) \\
+ a(\rho^{m-1}v^{m-1} + j^{m-1}, \widetilde{B_B w^m}, p_v^m) + a(\rho^{m-1}\widetilde{B_B w^{m-1}}, v^m, p_v^m) \\
+ 2(\eta^{m-1} D\widetilde{B_B w^m}, Dp_v^m) + (\widetilde{B_B w^m}\nabla\varphi^{m-1}, p_\varphi^m)\Bigg] = 0.
\end{aligned}
\tag{33}
$$

For smooth solutions we use the derivative with respect the velocity, the no-flux boundary condition for v^m as well as for μ^m and integration by parts to observe

$$
\begin{aligned}
(D_{u_B} L(u,\ldots), w) = \alpha\alpha_B \int_I (u_B, w)_{\mathbb{R}^{u_b}}\,dt \\
- \sum_{m=2}^{M}\int_{\partial\Omega} 2\eta^{m-1} Dp_v^m \cdot \nu_\Omega B_B w^m\,ds - \int_{\partial\Omega} 2\eta^1 Dp_v^1 \cdot \nu_\Omega B_B w^1\,ds
\end{aligned}
$$

and thus the optimality condition in a strong formulation is

$$
\begin{aligned}
\alpha\alpha_B \tau u_B^m - \left((2\eta^{m-1} Dp_v^m \cdot \nu_\Omega, g^l)_{H^{-1/2}(\partial\Omega),H^{1/2}(\partial\Omega)}\right)_{l=1}^{u_b} = 0 \in \mathbb{R}^{u_b} \quad \forall m = 2,\ldots,M, \\
\alpha\alpha_B \tau u_B^1 - (2\eta^1 Dp_v^1 \cdot \nu_\Omega, g^l)_{H^{-1/2}(\partial\Omega),H^{1/2}(\partial\Omega)} = 0 \in \mathbb{R}^{u_b}.
\end{aligned}
\tag{34}
$$

The derivative with respect to the initial condition u_I in a direction $w - u_I \in U_I$ is

$$
\begin{aligned}
(D_{u_I} L(u,\ldots), w - u_I)_{U_I^\star, U_I} = \frac{\alpha}{2}\alpha_I\left(\epsilon(\nabla u_I, \nabla(w-u_I)) + \epsilon^{-1}\int_\Omega W_u'(u_I)(w-u_I)\,dx\right) \\
- \frac{1}{2\tau}\left(\rho'(w-u_I)v^2, p_v^2\right) + \frac{1}{\tau}\left(\rho'(w-u_I)v^1, p_v^2\right) \\
- \frac{1}{2\tau}\left(\rho'(w-u_I)v^1, p_v^1\right) + \frac{1}{\tau}\left(\rho'(w-u_I)v^0, p_v^1\right) \\
+ (\mu^1\nabla(w-u_I), p_v^1) + (\rho'(w-u_I)K, p_v^1) \\
+ \frac{1}{\tau}((w-u_I), p_\varphi^1) - (v^0\nabla(w-u_I), p_\varphi^1) - \frac{\sigma}{\epsilon}(W_-''(u_I)(w-u_I), p_\mu^1) \geq 0.
\end{aligned}
\tag{35}
$$

We note that $u_I \in H^1(\Omega) \cap L^\infty(\Omega)$ and thus that there exists no gradient representation for $D_{u_I} L$. This is reflected later in our numerical approach.

Remark 3.10. From (32) we see, that in fact u_V has a discrete structure with respect to time, namely it is piecewise constant over time intervals, as the adjoint variable p_v is. The same holds for u_B.

4. The fully discrete setting

We next use finite elements to discretize the optimal control problem $\mathcal{P}$ in space. For this we use finite elements on locally adapted meshes. At time instance t_m, $m = 1,\ldots,M$ we use a quasi-uniform, triangulation of $\overline{\Omega}$ with NT_m triangles denoted by $\mathcal{T}_m = \{T_i\}_{i=1}^{NT_m}$ fulfilling $\overline{\Omega} = \bigcup_{i=1}^{NT_m} \overline{T}_i$.

On $\mathcal{T}_m$ we define the following finite element spaces:

$$\mathcal{V}_m^1 = \{v \in C(\mathcal{T}_m) \mid v|_T \in \mathcal{P}^1(T)\ \forall T \in \mathcal{T}_m\},$$
$$\mathcal{V}_m^2 = \{v \in C(\mathcal{T}_m)^n \mid v|_T \in \mathcal{P}^2(T)^n\ \forall T \in \mathcal{T}_m\},$$

where $\mathcal{P}^l(S)$ denotes the space of polynomials up to order l defined on S. We note that by construction $\mathcal{V}_m^1 \subset W^{1,\infty}(\mathcal{T}_m)$ and $\mathcal{V}_m^2 \subset W^{1,\infty}(\mathcal{T}_m)^n$ holds. We introduce the discrete analog to the space $H_\sigma(\Omega)$:

$$H_{\sigma,m} := \{v \in \mathcal{V}_m^2 \mid (\mathrm{div} v, q) = 0\ \forall q \in \mathcal{V}_m^1 \cap L^2(\Omega)\},$$

and

$$H_{0,\sigma,m} := \{v \in H_{\sigma,m} \mid \gamma(v) = 0\}.$$

We further introduce a linear H^1-stable projection operator $P^m : H^1(\Omega) \to \mathcal{V}_m^1$ satisfying

$$\|P^m v\|_{L^p(\Omega)} \le C\|v\|_{L^p(\Omega)}, \text{ and } \|\nabla P^m v\|_{L^r(\Omega)} \le C\|\nabla v\|_{L^r(\Omega)},$$

for $v \in H^1(\Omega)$ with $r \in [1,2]$ and $p \in [1,6]$ if $n = 3$, and $p \in [1,\infty)$ if $n = 2$ and

$$\|P^m v - v\|_{H^1(\Omega)} \to 0$$

for $h \to 0$ for $v \in H^2(\Omega)$ Typically examples are the Clément operator or, by restricting the preimage to $C(\overline{\Omega}) \cap H^1(\Omega)$, the Lagrangian interpolation operator.

We further introduce

$$\mathcal{V}_{m,b}^2 := \{v|_{\partial\Omega} \mid v \in \mathcal{V}_m^2, \int_{\partial\Omega} v|_{\partial\Omega} \cdot \nu_\Omega \, ds = 0\}$$

and define Π^m for $m = 1,\ldots,M$ as the $L^2(\partial\Omega)$ projection onto the trace space $\mathcal{V}_{m,b}^2$ of $\mathcal{V}_m^2$. This projection is used to incorporate the boundary data and fulfills $\|\Pi^m g - g\|_{L^2(\partial\Omega)} \to 0$ for all $g \in H^{1/2}(\partial\Omega)$ with $\int_{\partial\Omega} g \cdot \nu_\Omega \, ds = 0$.

Using these spaces we state the discrete counterpart of (13)–(18):

Let $u \in U$ and $v_0 \in H_\sigma \cap L^\infty(\Omega)^n$ be given.

Initialization for $m = 1$:

Set $\varphi_h^0 := u_I$, $v^0 := v_0$. Find $v_h^1 \in H_{\sigma,1}$, $\gamma(v_h^1) = \Pi^1(B_B u_B^1)$, $\varphi_h^1 \in \mathcal{V}_1^1$, $\mu_h^1 \in \mathcal{V}_1^1$ such that for all $w \in H_{0,\sigma,1}$, $\Psi \in \mathcal{V}_1^1$, $\Phi \in \mathcal{V}_1^1$ it holds:

$$\tau^{-1}\left(\frac{1}{2}(\rho_h^1 + \rho_h^0)v_h^1 - \rho_h^0 v^0, w\right) + a(\rho_h^1 v^0 + j_h^1, v_h^1, w)$$
$$+(2\eta_h^1 D v_h^1, Dw) - (\mu_h^1 \nabla\varphi_h^0 + \rho_h^0 g, w) - (B_V u_V^1, w) = 0, \tag{36}$$
$$\frac{1}{\tau}(\varphi_h^1 - P^1\varphi_h^0, \Psi) + (b\nabla\mu_h^1, \nabla\Psi) + (v^0\nabla\varphi_h^0, \Psi) = 0, \tag{37}$$
$$\sigma\epsilon(\nabla\varphi_h^1, \nabla\Phi) + \frac{\sigma}{\epsilon}(W_+'(\varphi_h^1) + W_-'(P^1\varphi_h^0), \Phi) - (\mu_h^1, \Phi) = 0, \tag{38}$$

where $j^1 := -\rho_\delta b\nabla\mu_h^1$.

Two-step scheme for $m > 1$:

Given $\varphi_h^{m-2} \in \mathcal{V}_{m-2}^1$, $\varphi_h^{m-1} \in \mathcal{V}_{m-1}^1$, $\mu_h^{m-1} \in \mathcal{V}_{m-1}^1$, $v_h^{m-1} \in H_{\sigma,m-1}$, find $v_h^m \in H_{\sigma,m}$, $\gamma(v_h^m) = \Pi^m(B_B u_B^m)$, $\varphi_h^m \in \mathcal{V}_m^1$,

$\mu_h^m \in \mathcal{V}_m^1$ such that for all $w \in H_{0,\sigma,m}$, $\Psi \in \mathcal{V}_m^1$, $\Phi \in \mathcal{V}_m^1$ it holds:

$$\tau^{-1}\left(\frac{1}{2}(\rho_h^{m-1}+\rho_h^{m-2})v_h^m - \rho_h^{m-2}v_h^{m-1}, w\right) + a(\rho_h^{m-1}v_h^{m-1} + j_h^{m-1}, v_h^m, w)$$

$$+(2\eta_h^{m-1}Dv_h^m, Dw) - (\mu_h^m \nabla\varphi_h^{m-1} + \rho_h^{m-1}g, w) - (B_V u_V^m, w) = 0, \tag{39}$$

$$\frac{1}{\tau}(\varphi_h^m - P^m\varphi_h^{m-1}, \Psi) + (b\nabla\mu_h^m, \nabla\Psi) + (v_h^m\nabla\varphi_h^{m-1}, \Psi) = 0, \tag{40}$$

$$\sigma\epsilon(\nabla\varphi_h^m, \nabla\Phi) + \frac{\sigma}{\epsilon}(W_+'(\varphi_h^m) + W_-'(P^m\varphi_h^{m-1}), \Phi) - (\mu_h^m, \Phi) = 0, \tag{41}$$

where $j_h^{m-1} := -\rho_\delta b\nabla\mu_h^{m-1}$.

We require bounds with respect to $W^{1,p}(\Omega)$-norms for the solution of (36)–(41) and prepare these with the following lemmas.

Lemma 4.1. *For all $1 < p < \infty$ there exists a continuous function $C(p)$, such that*

$$\|\nabla u\|_{L^p(\Omega)} \le C(p) \sup_{\substack{\eta\in L^q(\Omega),\eta\ne 0\\(\eta,1)=0}} \frac{(\nabla u, \nabla\eta)}{\|\nabla\eta\|_{L^q(\Omega)}},$$

where $\frac{1}{p}+\frac{1}{q}=1$. Further, from the generalized Poincaré inequality, [8, Thm. 8.16], we obtain $\|\eta\|_{W^{1,q}(\Omega)} \le C\|\nabla\eta\|_{L^q(\Omega)}$ and thus

$$\|\nabla u\|_{L^p(\Omega)} \le C(p) \sup_{\substack{\eta\in L^q(\Omega),\eta\ne 0\\(\eta,1)=0}} \frac{(\nabla u, \nabla\eta)}{\|\eta\|_{W^{1,q}(\Omega)}}.$$

Proof. The proof follows as in [11, Lem. 1.1] and uses L^p-stability for u shown in [24, Thm. 1.2]. □

Lemma 4.2. *For $v \in W^{1,p}(\Omega)$ let $Q_h v \in \mathcal{V}_m^1$ be defined by*

$$(\nabla Q_h v, \nabla w) = (\nabla v, \nabla w) \quad \forall w \in \mathcal{V}_m^1, \tag{42}$$

$$\int_\Omega Q_h v\,dx = \int_\Omega v\,dx. \tag{43}$$

Let $1 < p < \infty$. Then it holds

$$\|Q_h v\|_{W^{1,p}(\Omega)} \le C(p)\|v\|_{W^{1,p}(\Omega)}. \tag{44}$$

Proof. The proof follows the lines of [17, Ch. 8]. Combining it with the techniques provided in [11] and [48] allows also the treatment of Neumann boundary data. □

Lemma 4.3. *Let $u_h \in \mathcal{V}_m^1 \subset W^{1,q}(\Omega)$. Then it holds*

$$\|\nabla u_h\|_{L^p(\Omega)} \le C(p) \sup_{\substack{\eta_h\in V_m^1,\eta_h\ne 0\\(\eta,1)=0}} \frac{(\nabla u_h, \nabla\eta_h)}{\|\eta_h\|_{W^{1,q}(\Omega)}},$$

where $\frac{1}{p}+\frac{1}{q}=1$.

Proof. Directly follows by combining Lemma 4.1, the definition of $Q_h v$ in (43) and the stability estimate (44), compare [48, Thm. 2.3]. □

Theorem 4.4. *Let $v_0 \in H^1(\Omega)^n \cap L^\infty(\Omega)^n$, $u \in U$ be given. Then there exist unique $v_h^1 \in H_{\sigma,1}$, $\gamma(v_h^1) = \Pi^1(B_B u_B^1)$, $\varphi_h^1 \in \mathcal{V}_1^1$ and $\mu_h^1 \in \mathcal{V}_1^1$ solving (36)–(38). It further holds*

$$
\begin{aligned}
&\|\mu_h^1\|_{W^{1,3}(\Omega)} + \|\varphi_h^1\|_{W^{1,4}(\Omega)} + \|v_h^1\|_{H^1(\Omega)} \\
&\le C_1(v^0)C_2\left(\|u_I\|_{H^1(\Omega)}, \|B_V u_V^1\|_{L^2(\Omega)^n}, \|B_B u_B^1\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right),
\end{aligned}
$$

where the constants C_1, C_2 depend polynomially on their arguments and the system parameter, including ϵ^{-1}, but are independent of h.

Proof. For (37)–(38) the existence of a unique solution follows similar as in [33] by considering a suitable minimization problem. The additional term $v^0\nabla\varphi^0$ can be incorporated in a straightforward manner. Also the stability in H^1 is proven in [33].

To obtain the estimates of higher regularity we use Lemma 4.3. It holds (37)

$$
\begin{aligned}
C\|\mu_h^1\|_{W^{1,3}(\Omega)} &\le \|\nabla\mu_h^1\|_{L^3(\Omega)} + \|\mu_h^1\|_{L^3(\Omega)} \\
&\le \|\mu_h^1\|_{L^3(\Omega)} + C \sup_{\substack{v_h\in\mathcal{V}_m^1,(v_h,1)=0\\ \|v_h\|_{W^{1,\frac{3}{2}}(\Omega)}=1}} (\nabla\mu_h^1, \nabla v_h) \\
&\le C\|\mu_h^1\|_{H^1(\Omega)} + C\sup\left(\left|\frac{1}{\tau}(\varphi_h^1 - P^1\varphi_h^0, v_h)\right| + \left|(v^0\nabla\varphi_h^0, v_h)\right|\right) \\
&\le C\|\mu_h^1\|_{H^1(\Omega)} + C\sup\left(\|\varphi_h^1 - P^1\varphi_h^0\|_{L^2(\Omega)}\|v_h\|_{L^2(\Omega)} + \|v^0\nabla\varphi_h^0\|_{L^2(\Omega)^n}\|v_h\|_{L^2(\Omega)}\right) \\
&\le C\|\mu_h^1\|_{H^1(\Omega)} + C\|\varphi_h^1 - P^1\varphi_h^0\|_{L^2(\Omega)} + C\|v^0\nabla\varphi_h^0\|_{L^2(\Omega)^n} \\
&\le C\left(\|\mu_h^1\|_{H^1(\Omega)} + \|\varphi_h^1\|_{H^1(\Omega)} + \|\varphi_h^0\|_{H^1(\Omega)} + \|v^0\|_{L^\infty(\Omega)^n}\|\varphi_h^0\|_{H^1(\Omega)}\right)
\end{aligned}
\tag{45}
$$

which, together with the already known bound for $\|\mu_h^1\|_{H^1(\Omega)}$ states the bound on μ_h^1 in $W^{1,3}(\Omega)$. Note the continuous embedding $W^{1,\frac{3}{2}}(\Omega) \hookrightarrow L^2(\Omega)$ used for v_h.

For φ_h^1 we argue similarly and estimate

$$
\begin{aligned}
&C\|\varphi_h^1\|_{W^{1,4}(\Omega)} \\
&\le \|\varphi_h^1\|_{L^4(\Omega)} + C \sup_{\substack{v_h\in W^{1,\frac{4}{3}}(\Omega),(v_h,1)=0\\ \|v\|_{W^{1,\frac{4}{3}}(\Omega)}=1}} \left((\nabla\varphi_h^1, \nabla v_h)\right) \\
&\le C\|\varphi_h^1\|_{H^1(\Omega)} + C\sup\left(\left|(\mu_h^1, v_h)\right| + \left|\frac{\sigma}{\epsilon}(W'_+(\varphi_h^1) + W'_-(P^1\varphi_h^0), v_h)\right|\right) \\
&\le C\|\varphi_h^1\|_{H^1(\Omega)} + C\|\mu_h^1\|_{L^2(\Omega)} + C\sup\left[(1 + |\varphi_h^1|^{q-1}, |v_h|) + (1 + |P^1\varphi_h^0|^{q-1}, |v_h|)\right] \\
&\le C\|\varphi_h^1\|_{H^1(\Omega)} + C\|\mu_h^1\|_{L^2(\Omega)} \\
&\quad + C\left(\|1 + |\varphi_h^1|^{q-1}\|_{L^2(\Omega)} + \|1 + |P^1\varphi_h^0|^{q-1}\|_{L^2(\Omega)}\right)\sup\|v_h\|_{L^2(\Omega)} \\
&\le C\|\varphi_h^1\|_{H^1(\Omega)} + C\|\mu_h^1\|_{L^2(\Omega)} + C\left(1 + \|\varphi_h^1\|_{H^1(\Omega)} + \|\varphi_h^0\|_{H^1(\Omega)}\right).
\end{aligned}
$$

We note the continuous embeddings $W^{1,\frac{4}{3}}(\Omega) \hookrightarrow L^2(\Omega)$ and $H^1(\Omega) \hookrightarrow L^6(\Omega)$.

The existence of a unique solution for (36) and stability for v_h^1 then follows from Lax–Milgram's theorem as in Theorem 3.3 and considering a shifted system. □

Theorem 4.5. *For all $m = 2, \ldots, M$, let $u \in U$, $\varphi^{m-2} \in \mathcal{V}_{m-2}^1$, $\varphi^{m-1} \in \mathcal{V}_{m-1}^1$, $\mu^{m-1} \in \mathcal{V}_{m-1}^1$, $v^{m-1} \in H_{\sigma,m-1}$ be given. Then there exist unique $v_h^m \in H_{\sigma,m}$, $\gamma(v_h^m) = \Pi^m(B_B u_B^m)$, $\varphi_h^m \in \mathcal{V}_m^1$ and $\mu_h^m \in \mathcal{V}_m^1$ solving (39)–(41).*

It further holds

$$\begin{aligned}
&\|\mu_h^m\|_{W^{1,3}(\Omega)} + \|\varphi_h^m\|_{W^{1,4}(\Omega)} + \|v_h^m\|_{H^1(\Omega)^n} \\
&\le C\big(\|v_h^{m-1}\|_{H^1(\Omega)^n}, \|\mu_h^{m-1}\|_{W^{1,3}(\Omega)}, \|\varphi_h^{m-1}\|_{W^{1,4}(\Omega)}, \\
&\|B_V u_V^m\|_{L^2(\Omega)^n}, \|B_B u_B^m\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\Big),
\end{aligned}$$

where C depends polynomially on its arguments and the system parameters, including ϵ^{-1}, but is independent of h.

Proof. In [23] the existence of unique solutions to (39)–(41) together with bounds in $H^1(\Omega)$ on the solution is shown for the case $B_V u_V^m = 0$, $B_B u_B^m = 0$, using [51, Lem. II 1.4]. The volume force $B_V u_V^m$ is given data that enters the proof in a straightforward manner. The boundary data $B_B u_B^m$ can be incorporated by investigating a shifted system as in Theorem 3.4.

The estimates of higher regularity follow as in Theorem 4.4. There the bound for μ_h^1 relies on $L^\infty(\Omega)$ regularity of v^0, that is not available here. Instead in (45) we can use a $L^6(\Omega)$ bound for v_h^m that directly follows from the $H^1(\Omega)$ bound by Sobolov embedding, together with the $L^3(\Omega)$ bound for $\nabla\varphi_h^{m-1}$. □

Theorem 4.6. *Let $v^0 \in H^1(\Omega)^n \cap L^\infty(\Omega)$, $u \in U$ be given. Then there exist sequences $(v^m)_{m=1}^M \in (H_{\sigma,m})_{m=1}^M$, $(\varphi^m)_{m=1}^M, (\mu^m)_{m=1}^M \in (\mathcal{V}_m^1)_{m=1}^M$, such that (v^m, φ^m, μ^m) is the unique solution to (36)–(41) for $m = 1, \dots, M$. Moreover there holds*

$$\begin{aligned}
&\|(v_h^m)_{m=1}^M\|_{H^1(\Omega)} + \|(\mu_h^m)_{m=1}^M\|_{W^{1,3}(\Omega)} + \|(\varphi_h^m)_{m=1}^M\|_{W^{1,4}(\Omega)} \\
&\le C_1(v^0)C_2\left(\|u_I\|_{H^1(\Omega)}, \|(B_V u_V^m)_{m=1}^M\|_{L^2(\Omega)^n}, \|(B_B u_B^m)_{m=1}^M\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right).
\end{aligned}$$

Here the constants C_1, C_2 depend polynomially on their arguments and the system parameter, including ϵ^{-1} but are independent of h.

Proof. The existence of the solution for each time instance follows directly from Theorem 4.4 and Theorem 4.5. The stability estimate follows from iteratively applying the stability estimates from Theorem 4.4; □

Remark 4.7. The bounds with respect to higher norms are required in Section 5 for the limit process $h \to 0$.

To derive first order necessary optimality conditions we argue as in the case of the time discrete optimization problem and show that Newton's method can be used for solving the primal equation (36)–(41) on each time instance.

Theorem 4.8. *Newton's method can be used for finding the unique solution to* (36)–(41) *on each time instance.*

Proof. For $m = 1$ this is shown in [33]. For $m > 1$ we abbreviate equation (39)–(41) by

$$F((v_h^m, \varphi_h^m, \mu_h^m), (w, \Phi, \Psi)) = 0,$$

with a nonlinear operator $F : H_{\sigma,m} \times \mathcal{V}_m^1 \times \mathcal{V}_m^1 \to (H_{0,\sigma,m} \times \mathcal{V}_m^1 \times \mathcal{V}_m^1)^\star$. Then F is Fréchet differentiable, since all terms are linear beside the term W_+' which is Frechét differentiable by (A2). The derivative in a direction

$(\delta v, \delta\varphi, \delta\mu) \in H_{0,\sigma,m} \times \mathcal{V}_m^1 \times \mathcal{V}_m^1$ is given by

$$
\begin{aligned}
&\langle G(v_h^m, \varphi_h^m, \mu_h^m)(\delta v, \delta\varphi, \delta\mu), (w, \Phi, \Psi)\rangle :=\\
&\quad \frac{1}{\tau}\left(\frac{\rho^{m-1}+\rho^{m-2}}{2}\delta v, w\right) + a(\rho^{m-1}v^{m-1} + j^{m-1}, \delta v, w)\\
&\quad + (\eta^{m-1} D\delta v, Dw) - (\delta\mu \nabla\varphi^{m-1}, w)\\
&\quad + \frac{1}{\tau}(\delta\varphi, \Psi) + (b\nabla\delta\mu, \nabla\Psi) + (\delta v \nabla\varphi^{m-1}, \Psi)\\
&\quad + \sigma\epsilon(\nabla\delta\varphi, \nabla\Phi) + \frac{\sigma}{\epsilon}(W_+''(\varphi_h^m)\delta\varphi, \Phi) - (\delta\mu, \Phi).
\end{aligned}
$$

The existence of a solution $(\delta v, \delta\varphi, \delta\mu)$ can be shown following [23, Thm. 2], using Brouwer's fixpoint theorem. The boundedness of $(\delta v, \delta\varphi, \delta\mu)$ follows from the same proof. □

We next introduce the fully discrete analog to problem $(\mathcal{P})$.

$$
\begin{aligned}
\min_{u\in U} J((\varphi_h^m)_{m=1}^M, u) &= \frac{1}{2}\|\varphi_h^M - \varphi_d\|^2_{L^2(\Omega)}\\
&\quad + \frac{\alpha}{2}\left(\alpha_I\left(\int_\Omega \frac{\epsilon}{2}|\nabla u_I|^2 + \epsilon^{-1}W_u(u_I)\,dx\right)\right.\\
&\quad \left. + \alpha_V\|u_V\|^2_{L^2(0,T;\mathbb{R}^{u_v})} + \alpha_B\|u_B\|^2_{L^2(0,T;\mathbb{R}^{u_b})}\right)\\
\text{s.t. } (36) - (41).&
\end{aligned}
\tag{$\mathcal{P}_h$}
$$

We stress, that we do not discretize the control for the initial value. However for a practical implementation we need a discrete description for u_I. This will be discussed after deriving the optimality conditions, see Section 6.

Theorem 4.9 (Existence of an optimal discrete control)**.** *There exists at least one optimal control to $\mathcal{P}_h$.*

Proof. The claim follows from standard arguments, compare Theorem 3.7. □

We next state the fully discrete counterpart of the first order optimality conditions from Section 3.

For this we introduce adjoint variables $(p_{v,h}^m)_{m=1}^M \in (H_{0,\sigma,m})_{m=1}^M$, $(p_{\varphi,h}^m)_{m=1}^M \in (\mathcal{V}_m^1)_{m=1}^M$, and $(p_{\mu,h}^m)_{m=1}^M \in (\mathcal{V}^m)_{m=1}^M$. For convenience in the following we often write $v_h^m := v_{0,h}^m + \widetilde{B_B u_B^m}$.

By the same Lagrangian calculus as in Section 3 we obtain the following fully discrete optimality system.

Derivative with respect to the velocity

The derivative with respect to $v_{0,h}^m$ for $m = 2, \ldots, M$ into a direction $\tilde{v} \in \mathcal{V}_m^2$ is given by

$$
\begin{aligned}
&(D_{v_h^m} L(\ldots, v_h^m, \ldots), \tilde{v}) =\\
&\quad -\frac{1}{\tau}\left((\frac{\rho_h^{m-1}+\rho_h^{m-2}}{2}\tilde{v}, p_{v,h}^m) - (\rho_h^{m-1}\tilde{v}, p_{v,h}^{m+1})\right)\\
&\quad - a(\rho_h^m\tilde{v}, v_h^{m+1}, p_{v,h}^{m+1}) - a(\rho_h^{m-1}v_h^{m-1} + j_h^{m-1}, \tilde{v}, p_{v,h}^m)\\
&\quad - (2\eta_h^{m-1}D\tilde{v}, Dp_{v,h}^m) - (\tilde{v}\nabla\varphi_h^{m-1}, p_{\varphi,h}^m) = 0.
\end{aligned}
\tag{46}
$$

For $m = 1$ we get

$$
\begin{aligned}
&(D_{v_h^1} L(\ldots, v_h^1, \ldots), \tilde{v}) =\\
&\quad -\frac{1}{2\tau}((\rho_h^1 + \rho^0)\tilde{v}, p_{v,h}^1) + \frac{1}{\tau}(\rho^0\tilde{v}, p_{v,h}^2) - a(\rho_h^1\tilde{v}, v_h^2, p_{v,h}^2)\\
&\quad - a(\rho_h^1 v_h^0 + j_h^1, \tilde{v}, p_{v,h}^1) - (2\eta_h^1 D\tilde{v}, Dp_{v,h}^1) = 0.
\end{aligned}
\tag{47}
$$

Note that for notational convenience here we introduce artificial variables v_h^{M+1}, $p_{v,h}^{M+1}$, and set them to $v_h^{M+1} \equiv p_{v,h}^{M+1} \equiv 0$.

Derivative with respect to the chemical potential
The derivative with respect to the chemical potential for $m = 2, \ldots, M$ in a direction $\tilde{\mu} \in \mathcal{V}_m^1$ is

$$\begin{aligned}(D_{\mu_h^m} L(\ldots, \mu_h^m, \ldots), \tilde{\mu}) = \\ - a(j_\mu \tilde{\mu}, v_h^{m+1}, p_{v,h}^{m+1}) + (\tilde{\mu} \nabla \varphi_h^{m-1}, p_{v,h}^m) - (b \nabla \tilde{\mu}, \nabla p_{\varphi,h}^m) + (\tilde{\mu}, p_{\mu,h}^m) = 0.\end{aligned} \tag{48}$$

For $m = 1$ the equations is

$$\begin{aligned}(D_{\mu^1} L(\ldots, \mu^1, \ldots), \tilde{\mu}) = \\ - a(j_\mu \tilde{\mu}, v_h^2, p_{v,h}^2) - a(j_\mu^1 \tilde{\mu}, v_h^1, p_{v,h}^1) + (\tilde{\mu} \nabla u_I, p_{v,h}^1) \\ - (b \nabla \tilde{\mu}, \nabla p_{\varphi,h}^1) + (\tilde{\mu}, p_{\mu,h}^1) = 0.\end{aligned} \tag{49}$$

Here for $m = 1, \ldots, M$ we abbreviate $j_\mu^m \tilde{\mu} = -\rho_\delta b \nabla \tilde{\mu}$ and for notational convenience we introduce artificial variables v_h^{M+1} and $p_{v,h}^{M+1}$, and set them to $v_h^{M+1} \equiv p_{v,h}^{M+1} \equiv 0$.

Derivative with respect to the phase field
The derivative with respect to the phase field φ_h^m in a direction $\tilde{\varphi} \in \mathcal{V}_m^1$ is for $m = 2, \ldots, M$

$$\begin{aligned}(D_{\varphi_h^m} L(\ldots, \varphi_h^m, \ldots), \tilde{\varphi}) = \\ \delta_{mM}(\varphi_h^m - \varphi_d, \tilde{\varphi}) - \frac{1}{\tau}\left(\rho' \frac{v_h^{m+1} p_{v,h}^{m+1} + v_h^{m+2} p_{v,h}^{m+2}}{2}, \tilde{\varphi}\right) + \frac{1}{\tau}\left(\rho' v_h^{m+1} p_{v,h}^{m+2}, \tilde{\varphi}\right) \\ - a(\rho' \tilde{\varphi} v_h^m, v_h^{m+1}, p_{v,h}^{m+1}) - (2\eta' \tilde{\varphi} D v_h^{m+1}, D p_{v,h}^{m+1}) \\ + (\mu_h^{m+1} \nabla \tilde{\varphi}, p_{v,h}^{m+1}) + (\rho' \tilde{\varphi} g, p_{v,h}^{m+1}) \\ - \frac{1}{\tau}\left((\tilde{\varphi}, p_{\varphi,h}^m) - (P^{m+1} \tilde{\varphi}, p_{\varphi,h}^{m+1})\right) - (v_h^{m+1} \nabla \tilde{\varphi}, p_{\varphi,h}^{m+1}) \\ - \sigma\epsilon(\nabla \tilde{\varphi}, \nabla p_{\mu,h}^m) - \frac{\sigma}{\epsilon}(W_+''(\varphi_h^m)\tilde{\varphi}, p_{\mu,h}^m) - \frac{\sigma}{\epsilon}(W_-''(P^{m+1}\varphi_h^m) P^{m+1} \tilde{\varphi}, p_{\mu,h}^{m+1}) = 0.\end{aligned} \tag{50}$$

Here δ_{mM} denotes the Kronecker delta of m and M. For $m = 1$ we get

$$\begin{aligned}(D_{\varphi_h^1} L(\ldots, \varphi_h^1, \ldots), \tilde{\varphi}) = \\ - \frac{1}{\tau}(\frac{\rho'}{2}\tilde{\varphi}, v_h^2 p_{v,h}^2) - a(\rho' \tilde{\varphi} v_h^1, v_h^2, p_{v,h}^2) - a(\rho' \tilde{\varphi} v^0, v_h^1, p_{v,h}^1) \\ - (2\eta' \tilde{\varphi} D v_h^2, D p_{v,h}^2) - (2\eta' \tilde{\varphi} D v_h^1, D p_{v,h}^1) - (\mu_h^2 \nabla \tilde{\varphi} p_{v,h}^2) - (\rho' \tilde{\varphi} g, p_{v,h}^2) \\ + \frac{1}{\tau}(P^2 \tilde{\varphi}, p_{\varphi,h}^2) - (v_h^2 \nabla \tilde{\varphi}, p_{\varphi,h}^2) - \frac{\sigma}{\epsilon}(W_-''(P^2 \varphi_h^1) P^2 \tilde{\varphi}, p_{\mu,h}^2) \\ - \frac{1}{\tau}(\frac{\rho' \tilde{\varphi}}{2} v_h^1, p_{v,h}^1) - \frac{1}{\tau}(\tilde{\varphi}, p_{\varphi,h}^1) - \sigma\epsilon(\nabla \tilde{\varphi}, \nabla p_{\mu,h}^1) - \frac{\sigma}{\epsilon}(W_+''(\varphi_h^1)\tilde{\varphi}, p_{\mu,h}^1) = 0.\end{aligned} \tag{51}$$

Here for notational convenience we introduce artificial variables v_h^{M+1}, v_h^{M+2}, $p_{v,h}^{M+1}$, and $p_{v,h}^{M+2}$, and set them to zero.

Remark 4.10. We note that the projection operator P^m enters (50)–(51) acting on the test function $\tilde{\varphi}$.

Derivative with respect to the control
Finally we calculate the derivative with respect to the control for the three parts of the control space.

For a test direction $w \in U_V$ we have

$$(D_{u_V} L(u,\dots), w) = \alpha\alpha_V \int_I (u_V, w)_{\mathbb{R}^{u_v}}\, dt + \sum_{m=1}^{M} (B_V w^m, p_{v,h}^m)_{L^2(\Omega)} = 0,$$

and thus the optimality condition is

$$\alpha\tau\alpha_V u_V^m + B_V^\star p_{v,h}^m = 0 \in \mathbb{R}^{u_v} \quad m = 1,\dots,M. \tag{52}$$

Here $B_V^\star p_v^m$ is defined as

$$B_V^\star p_v^m := ((f_l, p_{v,h}^m)_{L^2(\Omega)^n})_{l=1}^{u_v}.$$

Concerning the derivative with respect to u_B we have for a test function $w \in U_B$

$$\begin{aligned}
(D_{u_B} L(u,\dots), w) &= \alpha\alpha_B \int_I (u_B, w)_{\mathbb{R}^{u_b}}\, dt - \tau^{-1}\left(\frac{\rho_h^1 + \rho^0}{2}\widetilde{B_B w^1}, p_{v,h}^1\right) \\
&- a(\rho_h^1 v^0 + j_h^1, \widetilde{B_B w^1}, p_{v,h}^1) - 2(\eta_h^1 D\widetilde{B_B w^1}, Dp_{v,h}^1) \\
&- \sum_{m=2}^{M}\left[\tau^{-1}\left(\frac{\rho_h^{m-1} + \rho_h^{m-2}}{2}\widetilde{B_B w^m}, p_{v,h}^m\right) - \left(\rho_h^{m-2}\widetilde{B_B w^{m-1}}, p_{v,h}^m\right)\right. \\
&+ a(\rho_h^{m-1} v_h^{m-1} + j_h^{m-1}, \widetilde{B_B w^m}, p_{v,h}^m) + a(\rho_h^{m-1}\widetilde{B_B w^{m-1}}, v_h^m, p_{v,h}^m) \\
&\left. + 2(\eta_h^{m-1} D\widetilde{B_B w^m}, Dp_{v,h}^m) + (\widetilde{B_B w^m}\nabla\varphi_h^{m-1}, p_{\varphi,h}^m)\right] \\
&=: \alpha\alpha_B \int_I (u_B, w)_{\mathbb{R}^{u_b}}\, dt + F_h(w) = 0.
\end{aligned} \tag{53}$$

Here $F_h(w)$ abbreviates the action of the discrete normal derivative of $p_{v,h}$, see e.g. [41].

The derivative with respect to the initial condition u_I in any direction $w - u_I \in U_I$ is

$$\begin{aligned}
(D_{u_I} L(u,\dots), w - u_I)_{U_I^\star, U_I} &= \frac{\alpha}{2}\alpha_I\left(\epsilon(\nabla u_I, \nabla(w - u_I)) + \epsilon^{-1}\int_\Omega W_u'(u_I)(w - u_I)\, dx\right) \\
&- \frac{1}{2\tau}\left(\rho'(w - u_I)v_h^2, p_{v,h}^2\right) + \frac{1}{\tau}\left(\rho'(w - u_I)v_h^1, p_{v,h}^2\right) \\
&- \frac{1}{2\tau}\left(\rho'(w - u_I)v_h^1, p_{v,h}^1\right) + \frac{1}{\tau}\left(\rho'(w - u_I)v^0, p_{v,h}^1\right) \\
&+ (\mu_h^1\nabla(w - u_I), p_{v,h}^1) + (\rho'(w - u_I)K, p_{v,h}^1) \\
&+ \frac{1}{\tau}((w - u_I), p_{\varphi,h}^1) - (v^0\nabla(w - u_I), p_{\varphi,h}^1) - \frac{\sigma}{\epsilon}(W_-''(u_I))(w - u_I), p_{\mu,h}^1) \geq 0,
\end{aligned} \tag{54}$$

and this inequality holds for all $w \in U_I$.

Remark 4.11. We use the finite element space $\mathcal{V}_1^1$ for the representation of u_I.

5. The limit $h \to 0$

We next investigate the limit $h \to 0$ for problem $\mathcal{P}_h$. Let $u^\star, \varphi^\star$ denote a solution to $\mathcal{P}$ and u_h, φ_h denote a solution to $\mathcal{P}_h$. Since u_h, φ_h is a minimizer for J in the discrete setting, we have $J(u_h, \varphi_h) \leq J(P_h u^\star, P_h\varphi^\star) \leq$

$CJ(u^\star,\varphi^\star) = Cj$, where P_h denotes any H^1-stable projection onto the discrete spaces. Thus

$$\begin{aligned}\frac{1}{2}\|\varphi_h^M - \varphi_d\|^2 + \frac{\alpha}{2}\Bigg(\alpha_I \int_\Omega \frac{\epsilon}{2}|\nabla u_{I,h}|^2 + \epsilon^{-1}W_u(u_{I,h})\,dx \\ + \alpha_V \|u_{B,h}\|^2_{L^2(0,T;\mathbb{R}^{u_v})} + \alpha_B\|u_{V,h}\|^2_{L^2(0,T;\mathbb{R}^{u_b})}\Bigg) \le Cj.\end{aligned} \tag{55}$$

Note that the mean value of $u_{I,h}$ is fixed and thus by Poincarés inequality we have $\|u_{I,h}\|_{H^1(\Omega)} \le C(1+\|\nabla u_{I,h}\|)$.

Thus from (55) we obtain the following bounds uniform in h:

$$\|u_{I,h}\|_{H^1(\Omega)} + \|u_{B,h}\|_{L^2(0,T;\mathbb{R}^{u_v})} + \|u_{V,h}\|_{L^2(0,T;\mathbb{R}^{u_b})} \le C.$$

Using Theorem 4.6 we further get the bounds

$$\|(v_h^m)_{m=1}^M\|_{H^1(\Omega)^n} + \|(\mu_h^m)_{m=1}^M\|_{W^{1,3}(\Omega)} + \|(\varphi_h^m)_{m=1}^M\|_{W^{1,4}(\Omega)} \le C.$$

Using Lax-Milgram's theorem and the above bounds we further obtain bounds

$$\|(p_{v,h}^m)_{m=1}^M\|_{H^1(\Omega)^n} + \|(p_{\varphi,h}^m)_{m=1}^M\|_{H^1(\Omega)} + \|(p_{\mu,h}^m)_{m=1}^M\|_{H^1(\Omega)} \le C$$

for the adjoint variables.

Now there exist $u_I^\star \in H^1(\Omega)$, $u_V^\star \in L^2(0,T;\mathbb{R}^{u_v})$, $u_B^\star \in L^2(0,T;\mathbb{R}^{u_b})$ such that

$$u_{I,h} \rightharpoonup u_I^\star, \quad u_{V,h} \rightharpoonup u_V^\star, \quad u_{B,h} \rightharpoonup u_B^\star.$$

There further exist $(v^{m,\star})_{m=1}^M \in (H^1(\Omega)^n)^M$, $(\varphi^{m,\star})_{m=1}^M \in W^{1,4}(\Omega)^M$, and $(\mu^{m,\star})_{m=1}^M \in W^{1,3}(\Omega)^M$ such that

$$v_h^m \rightharpoonup v^{m,\star}, \quad \varphi_h^m \rightharpoonup \varphi^{m,\star}, \quad \mu_h^m \rightharpoonup \mu^{m,\star} \quad \forall m = 1,\dots,M.$$

And there further exist $(p_v^{m,\star})_{m=1}^M \in H^1(\Omega)^M$, $(p_\varphi^{m,\star})_{m=1}^M \in H^1(\Omega)^M$, and $(p_\mu^{m,\star})_{m=1}^M \in H^1(\Omega)^M$ such that

$$p_{v,h}^m \rightharpoonup p_v^{m,\star}, \quad p_{\varphi,h}^m \rightharpoonup p_\varphi^{m,\star}, \quad p_{\mu,h}^m \rightharpoonup p_\mu^{m,\star} \quad \forall m = 1,\dots,M.$$

Now let us proceed to the limit in the fully discrete optimality system. To this end we will especially show the following strong convergence results

$$\begin{aligned}\varphi_h^m &\to \varphi^m \quad \text{in } H^1(\Omega),\\ \mu_h^m &\to \mu^m \quad \text{in } W^{1,3}(\Omega),\\ v_h^m &\to v^m \quad \text{in } H_\sigma(\Omega),\\ u_{I,h} &\to u_I \quad \text{in } H^1(\Omega),\end{aligned}$$

for $m = 1,\dots,M$.

The limit $h \to 0$ in the primal equation

The convergence of (41) to (18) and of (38) to (15) follows directly from the proposed weak convergences together with the strong convergence $\varphi_h^m \to \varphi^m$ in L^∞ obtained by compact Sobolev embedding. To obtain strong convergence in $H^1(\Omega)$ we argue as in the proof of Theorem 4.4.

Let $B : H^1(\Omega)\times H^1(\Omega) \to \mathbb{R}$ denote the coercive bilinear form $B(u,v) = \sigma\epsilon(\nabla u,\nabla v)+(u,v)$ and let $Q_h\varphi^1 \in \mathcal{V}_1^1$ denote the projection of φ^1 onto $\mathcal{V}_1^1$ with respect to B fulfilling $\|Q_h\varphi^1 - \varphi^1\|_{H^1(\Omega)} \to 0$ for $h \to 0$, since $\varphi^1 \in H^2(\Omega)$.

Then it holds

$$\|\varphi_h^1-\varphi^1\|_{H^1(\Omega)} \le \|\varphi_h^1-Q_h\varphi^1\|_{H^1(\Omega)} + \|Q_h\varphi^1-\varphi^1\|_{H^1(\Omega)},$$

and

$$\begin{aligned}
&C\|\varphi_h^1-Q_h\varphi^1\|^2_{H^1(\Omega)}\\
&\le B(\varphi_h^1-Q_h\varphi^1,\varphi_h^1-Q_h\varphi^1) = B(\varphi_h^1-\varphi^1,\varphi_h^1-Q_h\varphi^1)\\
&\le |(\mu_h^1-\mu^1,\varphi_h^1-Q_h\varphi^1)| + \|\varphi_h^1-\varphi^1\|_{L^2(\Omega)}\|\varphi_h^1-Q_h\varphi^1\|_{L^2(\Omega)}\\
&\quad+\frac{\sigma}{\epsilon}|(W'_+(\varphi_h^1)-W'_+(\varphi^1),\varphi_h^1-Q_h\varphi^1)| + \frac{\sigma}{\epsilon}|(W'_-(P^1\varphi_h^0)-W'_-(\varphi^0),\varphi_h^1-Q_h\varphi^1)|\\
&\le \|\mu_h^1-\mu^1\|_{L^2(\Omega)}\|\varphi_h^1-Q_h\varphi^1\|_{L^2(\Omega)} + \|\varphi_h^1-\varphi^1\|_{L^2(\Omega)}\|\varphi_h^1-Q_h\varphi^1\|_{L^2(\Omega)}\\
&\quad+\frac{\sigma}{\epsilon}\|W'_+(\varphi_h^1)-W'_+(\varphi^1)\|_{L^{5/3}(\Omega)}\|\varphi_h^1-Q_h\varphi^1\|_{L^{5/2}(\Omega)}\\
&\quad+\frac{\sigma}{\epsilon}\|W'_-(P^1\varphi_h^0)-W'_-(\varphi^0)\|_{L^{5/3}(\Omega)}\|\varphi_h^1-Q_h\varphi^1\|_{L^{5/2}(\Omega)}.
\end{aligned}$$

Using the Sobolev embedding $H^1(\Omega)\hookrightarrow L^p(\Omega)$, $p\le 6$ and dividing by $\|\varphi_h^1-Q_h\varphi^1\|_{H^1(\Omega)}$ we obtain

$$\begin{aligned}
C\|\varphi_h^1-Q_h\varphi^1\|_{H^1(\Omega)} \le& \|\mu_h^1-\mu^1\|_{L^2(\Omega)} + \|\varphi_h^1-\varphi^1\|_{L^2(\Omega)}\\
&+\frac{\sigma}{\epsilon}\|W'_+(\varphi_h^1)-W'_+(\varphi^1)\|_{L^{5/3}(\Omega)} + \frac{\sigma}{\epsilon}\|W'_-(P^1\varphi_h^0)-W'_-(\varphi^0)\|_{L^{5/3}(\Omega)}.
\end{aligned}$$

The first two terms on the right converge to zero by the compact embedding $H^1(\Omega)\hookrightarrow L^2(\Omega)$. Since $|W'_+(\varphi_h^1)|^{5/3}\le C(1+|\varphi_h^1|^3)^{5/3}\in L^5(\Omega)\subset L^1(\Omega)$, by using Assumption (A3), the third term converges by Lebesgue's generalized convergence theorem [8, Thm. 3.25]. The same argument holds for the last term, where we additionally use the stability of P^1 with respect to $L^5(\Omega)$. The same arguments apply for the case $m>1$.

The convergence of equation (40) to (17) and (37) to (14) is shown using the strong convergence $v_h^m\to v^m$ in $L^3(\Omega)$ together with weak convergence $\nabla\varphi_h^{m-1}\rightharpoonup\nabla\varphi^{m-1}$ in $L^2(\Omega)$ yielding weak convergence of the transport term $v_h^m\nabla\varphi_h^{m-1}$ in $L^{6/5}$. For $m=1$ $v^0\nabla\varphi_h^0$ converges weakly in $L^2(\Omega)$. Further, strong convergence $\mu_h^m\to\mu^m$ in $H^1(\Omega)$ follows as above.

To show strong convergence in $W^{1,3}$ it is thus sufficient to show strong convergence for $\nabla\mu_h^1\to\nabla\mu^1$ in $L^3(\Omega)$. We define $Q_hv\in\mathcal{V}_1^1$ by

$$\begin{aligned}
(\nabla(Q_hv-v),\nabla w_h)=0 \quad \forall w_h\in\mathcal{V}_1^1,\\
(Q_hv,1)=(v,1),
\end{aligned}$$

satisfying $\|Q_hv\|_{W^{1,\frac{3}{2}}(\Omega)}\le C\|v\|_{W^{1,\frac{3}{2}}(\Omega)}$, Lemma 4.2.

We adapt the idea from Theorem 4.4 and proceed

$$
\begin{aligned}
&C\|\nabla\mu_h^1 - \nabla\mu^1\|_{L^3(\Omega)} \\
&\le \sup_{\substack{v\in W^{1,\frac{3}{2}}(\Omega),(v,1)=0\\ \|v\|_{W^{1,\frac{3}{2}}(\Omega)}=1}} (\nabla(\mu_h^1-\mu^1),\nabla v) = \sup\left[(\nabla(\mu_h^1-\mu^1),\nabla Q_h v) + (\nabla(\mu_h^1-\mu^1),\nabla(v-Q_h v))\right] \\
&\le \sup\left[(\nabla(\mu_h^1-\mu^1),\nabla Q_h v) + (\nabla\mu^1,\nabla(Q_h v - v))\right] \\
&\le C\sup\left[|\tau^{-1}(\varphi_h^1-\varphi^1,Q_h v)| + |\tau^{-1}(P^1\varphi_h^0-\varphi^0,Q_h v)| + |(v^0\nabla\varphi_h^0 - v^0\nabla\varphi^0,Q_h v)\right. \\
&\left.+|\tau^{-1}(\varphi^1-\varphi^0,Q_h v - v)| + |(v^0\nabla\varphi^0,Q_h v - v)|\right] \\
&\le C\left[\|\varphi_h^1-\varphi^1\|_{L^2(\Omega)} + \|P^1\varphi_h^0-\varphi^0\|_{L^2(\Omega)}\right. \\
&\left.+\|\varphi^1-\varphi^0\|_{L^2(\Omega)}\sup\|Q_h v - v\|_{L^2(\Omega)} + \|v^0\nabla\varphi^0\|_{L^2(\Omega)}\sup\|Q_h v - v\|_{L^2(\Omega)}\right] \\
&+ C\sup|(v^0\nabla Q_h v,\varphi_h^0-\varphi^0)| \\
&\le C\left[\|\varphi_h^1-\varphi^1\|_{L^2(\Omega)} + \|P^1\varphi_h^0-\varphi^0\|_{L^2(\Omega)}\right. \\
&\left.+\|\varphi^1-\varphi^0\|_{L^2(\Omega)}\sup\|Q_h v - v\|_{L^2(\Omega)} + \|v^0\nabla\varphi^0\|_{L^2(\Omega)}\sup\|Q_h v - v\|_{L^2(\Omega)}\right] \\
&+ C\|v^0\|_{L^\infty(\Omega)}\|\varphi_h^0-\varphi^0\|_{L^2(\Omega)}.
\end{aligned}
$$

Note that we used integration by parts to deal with the transport term. From the Hölder and Sobolev inequalities it follows

$$\|Q_h v - v\|_{L^2(\Omega)}^2 \le \|Q_h v - v\|_{L^{\frac{3}{2}}(\Omega)}\|Q_h v - v\|_{L^3(\Omega)}.$$

The last term is bounded due to the fact, that $\|v\|_{W^{1,\frac{3}{2}}(\Omega)} \le 1$ and Q_h is stable in $W^{1,\frac{3}{2}}(\Omega)$. Since $\|Q_h v - v\|_{L^{\frac{3}{2}}(\Omega)} \le Ch\|v\|_{W^{1,\frac{3}{2}}(\Omega)}$ we obtain $\|Q_h v - v\|_{L^2(\Omega)} \to 0$ for $h \to 0$ and thus the strong convergence of $\nabla\mu_h$ in $L^3(\Omega)$. If $m > 1$ we can use the strong convergence $\varphi_h^{m-1} \to \varphi^{m-1}$ in $H^1(\Omega) \hookrightarrow L^6(\Omega)$ together with $\|v_h^m\|_{L^6(\Omega)} \le C$ to treat the transport term.

Next we consider the convergence of (39) to (16) and (36) to (13). Here the convergence $(\eta_h^{m-1}Dv_h^m : Dw) \to (\eta^{m-1}Dv^m : Dw)$ follows from the strong convergence $\varphi_h^{m-1} \to \varphi^{m-1}$ in $L^\infty(\Omega)$ (by compact embedding $W^{1,4}(\Omega) \hookrightarrow L^\infty(\Omega)$) and the weak convergence $Dv_h^m \rightharpoonup Dv^m$ in $L^2(\Omega)$. The convergence of the trilinear form is obtained by using the just shown strong convergence $\nabla\mu_h^m \to \nabla\mu^m$ in $L^3(\Omega)$ together with the weak convergence of $v_h^m \rightharpoonup v^m$ in $L^6(\Omega)$.

Let us finally show strong convergence $v_h^m \to v^m$ in $H^1(\Omega)^n$ for $m = 1,\dots,M$ Let $B : H_{0,\sigma,1} \times H_{0,\sigma,1} \to \mathbb{R}$ denote the coercive bilinear form $B(u,v) = 2(\eta_h^1 Du : Dv) + (u,v)$. The coercivity of B follows from Korn's inequality. Let $w_h \in H_{\sigma,1}$ denote the Ritz projection of v^1 in H_σ with boundary values $\gamma(v_h^1) \equiv \Pi(B_B u_B^1)$. Then $w_h - v^1 \to 0$ in $H^1(\Omega)^n$. Since $v_h^1 \rightharpoonup v^1$ in $H^1(\Omega)^n$ we find $w_h - v_h^1 \rightharpoonup 0$ in $H^1(\Omega)^n$, and $w_h - v_h^1 \in H_{0,\sigma,1}$. We thus may estimate

$$\|v_h^1 - v^1\|_{H^1(\Omega)^n} \le \|v_h^1 - w_h\|_{H^1(\Omega)^n} + \|w_h - v^1\|_{H^1(\Omega)^n}.$$

Now we proceed with

$$
\begin{aligned}
C\|v_h^1 - w_h\|^2_{H^1(\Omega)^n} &\le B(v_h^1 - w_h, v_h^1 - w_h) = B(v_h^1, v_h^1 - w_h) - B(w_h, v_h^1 - w_h)\\
&\le (B_V u^1_{V,h}, v_h^1 - w_h) + (\mu_h^1 \nabla\varphi_h^0, v_h^1 - w_h) + (\rho_h^0 g, v_h^1 - w_h)\\
&- a(\rho_h^1 v^0 + j_h^1, v_h^1, v_h^1 - w_h) - \tau^{-1}\left(\frac{\rho_h^1 + \rho_h^0}{2} v_h^1 - \rho_h^0 v^0, v_h^1 - w_h\right)\\
&+ (v_h^1, v_h^1 - w_h) - 2(\eta_h^1 D w_h : D(v_h^1 - w_h)) - (w_h, v_h^1 - w_h)\\
&\le \|B_V u^1_{V,h}\|_{L^2(\Omega)} \|v_h^1 - w_h\|_{L^2(\Omega)} + \|\mu_h^1 \nabla\varphi_h^0\|_{L^{\frac{3}{2}}(\Omega)} \|v_h^1 - w_h\|_{L^3(\Omega)}\\
&+ \|\rho_h^0 g\|_{L^2(\Omega)^n} \|v_h^1 - w_h\|_{L^2(\Omega)}\\
&+ |a(\rho_h^1 v^0 + j_h^1, v_h^1, v_h^1 - w_h)|\\
&+ \tau^{-1}\|\frac{1}{2}(\rho_h^1 + \rho_h^0) v_h^1 - \rho_h^0 v^0\|_{L^2(\Omega)} \|v_h^1 - w_h\|_{L^2(\Omega)}\\
&+ \|v_h^1 - w_h\|^2_{L^2(\Omega)} + |2(\eta_h^1 D w_h : D(v_h^1 - w_h))|.
\end{aligned}
$$

Now $|(\eta_h^1 D w_h^1 : D(v_h^1 - w_h))| \to 0$ for $h \to 0$ since $\eta_h^1 D w_h \to \eta^1 D v^1$ in $L^2(\Omega)$ and $D(v_h^1 - w_h) \rightharpoonup 0$ in $L^2(\Omega)$, and thus beside the trilinear form all terms directly vanish for $h \to 0$.

For the trilinear form we use the antisymmetry $a(\cdot, v_h^1 - w_h, v_h^1 - w_h) = 0$ and proceed

$$
\begin{aligned}
\left|a(\rho_h^1 v^0 + j_h^1, v_h^1, v_h^1 - w_h)\right| &= \left|a(\rho_h^1 v^0 + j_h^1, w_h, v_h^1 - w_h)\right|\\
&\le \left|\frac{1}{2}((\rho_h^1 v^0 + j_h^1)\nabla w_h, v_h^1 - w_h)\right| + \left|\frac{1}{2}((\rho_h^1 v^0 + j_h^1)\nabla(v_h^1 - w_h), w_h)\right|.
\end{aligned}
$$

We note the strong convergence $\rho_h^1 v^0 + j_h^1 \to \rho^1 v^0 + j^1$ in $L^3(\Omega)$ and for the first term we additionally use the strong convergence of $\nabla w_h \to \nabla v^1$ in $L^2(\Omega)$ and the weak convergence $v_h^1 - w_h \rightharpoonup 0$ in $L^6(\Omega)$ to observe that the first term tends to zero. For the second term we proceed vice versa and use the strong convergence $w_h \to v_1$ in $L^2(\Omega)$ and the weak convergence $\nabla(v_h^1 - w_h) \rightharpoonup 0$ in $L^2(\Omega)$ to observe that also the second term tends to zero for $h \to 0$.

For $m > 1$ we use $\rho_h^{m-1} \to \rho^{m-1}$ in $L^\infty(\Omega)$ to again obtain the strong convergence $\rho_h^{m-1} v_h^{m-1} + j_h^{m-1} \to \rho^{m-1} v^{m-1} + j^{m-1}$ in $L^3(\Omega)$.

The limit $h \to 0$ in the dual equation

The convergence of (46) and (47) to (26) and (27), i.e. the adjoint Navier–Stokes equation, is shown as in the primal equation using the strong convergence of φ_h^m in $L^\infty(\Omega)$ and μ_h^m in $W^{1,3}(\Omega)$ to show convergence of the trilinear form and of the diffusion term.

The convergence of (48) and (49) to (28) and (29) uses strong convergence of $p_{v,h}^{m+1}$ in $L^4(\Omega)$ and of v_h^{m+1} in $L^6(\Omega)$, where the additional regularity for v_h is required.

The convergence of (50) and (51) to (30) and (31) also follows directly using the above shown strong convergence of the primal variables. Especially for the term $(\eta' \tilde{\varphi} D v_h^{m+1} : D p_{v,h}^{m+1})$ we need the strong convergence $v_h^{m+1} \to v^{m+1}$ in $H^1(\Omega)$.

The limit $h \to 0$ in the derivative w.r.t. the control

The convergence of (52) to (32) is shown using the strong convergence $p_{v,h}^m$ in $L^2(\Omega)$.

The convergence of (53) to (33) is shown using the various strong convergence results.

Finally we show the convergence of (54) to (35). Since $J(u_h, \varphi_h) \to J(u^\star, \varphi^\star)$, we observe convergence $\|\nabla u_{I,h}\|_{L^2(\Omega)} \to \|\nabla u_I^\star\|_{L^2(\Omega)}$. Together with Poincaré's inequality and the weak convergence $u_{I,h} \rightharpoonup u_I^\star$ in $H^1(\Omega)$ we observe strong convergence $u_{I,h} \to u_I^\star$ in $H^1(\Omega)$. The convergence (54) to (35) now readily follows.

6. Numerical examples

In this section we show numerical results for the optimal control problem $\mathcal{P}_h$. The implementation is done in `C++` using the finite element toolbox FEniCS [47] together with the PETSc linear algebra backend [10] and the linear solver MUMPS [9]. For the adaptation of the spatial meshes the toolbox ALBERTA [50] is used. The minimization problem is solved by steepest descent method. If the initial phase field is not used as control, we use the GNU scientific library [1], if the initial value is used as control we use a self written implementation using the H^1 regularity of the control u_1.

Let us next define some data, that is used throughout all examples. We use $\rho(\varphi) = \frac{\rho_2-\rho_1}{2}\varphi + \frac{\rho_1+\rho_2}{2}$ and $\eta(\varphi) = \frac{\eta_2-\eta_1}{2}\varphi + \frac{\eta_1+\eta_2}{2}$, where ρ_1, ρ_2 and η_1, η_2 depend on the actual example. For the free energy we always use (9), with $s = 1e4$, and the mobility is set to $b \equiv \epsilon/500$.

6.1. **The adaptive concept**

For the construction of the spatially adapted meshes we use the error indicators that are constructed in [23] for the primal equation and use the series of meshes that we construct for the primal equation also for the dual equation. This means that we use classical residual based error estimation to obtain suitable error indicators. We note that following [18] the cell-wise residuals for the Cahn–Hilliard equation can be subsumed to the edge-wise error indicators. We further note that from our numerical tests we obtain that the cell-wise residuals of the momentum equation is much smaller than the edge-wise indicators, while it turns out to be very expensive to evaluate. Thus we neglect this term. The final error indicator is the cell-wise sum of the jumps of the normal derivatives of the phase field variable, the chemical potential and the velocity field over the cell boundary. The final adaptation scheme for the primal equation is a Dörfler marking scheme based on this indicator, see e.g. [20, 23].

For the Dörfler marking we set the largest cell volume to $V_{max} = 0.0003$, while the smallest cell volume is set to $V_{min} = \frac{1}{2}\left(\frac{\pi\epsilon}{8}\right)^2$ which results in 8 triangles across the interface of thickness $\mathcal{O}(\pi\epsilon)$.

Concerning the temporal resolution, we stress that we did not discretize the control u_V and u_B with respect to time, i.e. we use the variational discretization approach from [38]. Thus we can adapt the time step size during the optimization to fulfill a CFL-condition without changing the actual control space. Thus we start with a given large time step size τ and reduce this steps size whenever the CFL-condition $\max_T \frac{|y^m|_T|\tau}{\mathrm{diam}(T)} \le 1$ is violated for any $m = 1, \ldots, M$ by halven τ.

6.2. **A rising bubble**

In this example investigate the pure boundary control $\alpha_V \equiv \alpha_I \equiv 0$. Here we use $u_I = \varphi_0$ as given data that we represent on a adapted mesh using the proposed adaptive concept.

We investigate the example of a rising bubble, compare [44] and use the parameters from the benchmark paper [42], i.e. $\rho_1 = 1000$, $\rho_2 = 100$, $\eta_1 = 10$, $\eta_2 = 1$. The surface tension is 24.5 which due to our choice of free energy corresponds to $\sigma = 15.5972$. The gravitational constant is $g = (0, -0.981)^t$ and the computational domain is $\Omega = (0,1) \times (0,1.5)$. The time interval is $I = [0, 1.0]$ and we start with a step size $\tau = 5e-3$, that is refined to $\tau = 2.5e-3$ throughout the optimization.

The initial phase field is given by

$$\varphi_0(x) = \begin{cases} \sin((\|x - M_1\| - r)/\epsilon) & \text{if } |\|x - M_1\| - r|/\epsilon \le \pi/2, \\ \mathrm{sign}(\|x - M_1\| - r) & \text{else}, \end{cases} \tag{56}$$

with $M_1 = (0.5, 0.75)^t$ and $r = 0.25$. The desired phase field is given by the same expression but with $M_1 = (0.5, 0.5)^t$. Thus we aim to move a bubble to the bottom without changing its shape.

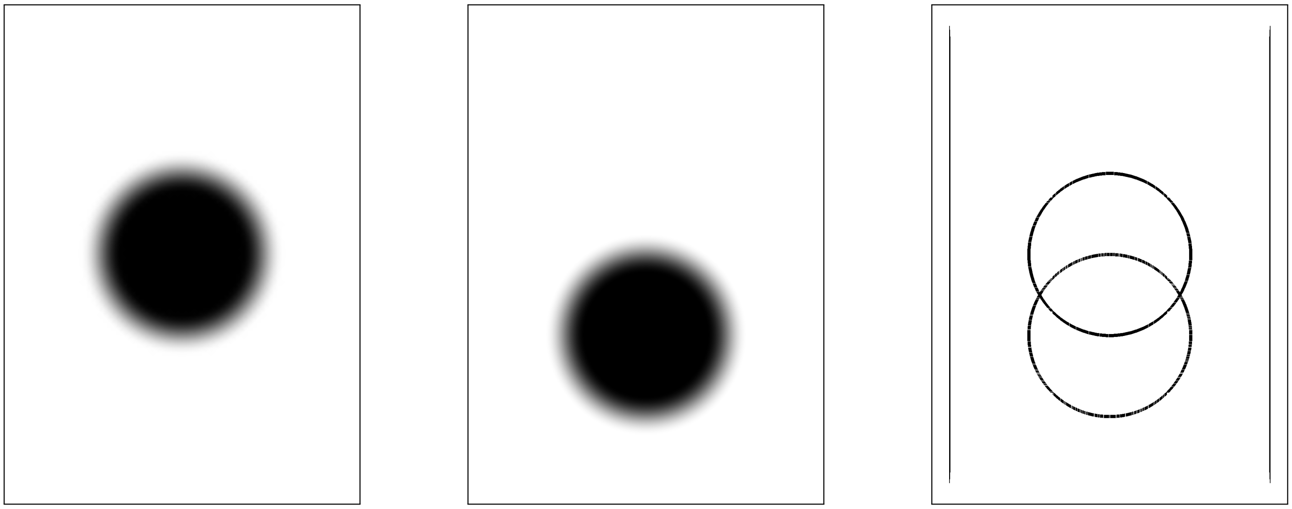

FIGURE 1. The initial phase field φ_0 (left), the desired phase field φ_d (middle) and the control areas together with the zero-level lines of φ_0 and φ_d (right) for the rising bubble example. Note that each of the control areas contains 10 controls of the type $f[m,\xi,c](x)$ that point tangential to $\partial\Omega$ with overlapping support.

Concerning the ansatz functions for the operator B_B we introduce the vector field

$$(f[m,\xi,c](x))_i = \begin{cases} \cos\left((\pi/2)\|\xi^{-1}(x-m)\|\right)^2 & \text{if } c \equiv i \text{ and } \|\xi^{-1}(x-m)\| \le 1, \\ 0 & \text{else.} \end{cases}$$

This describes an approximation to the Gaussian bell with local support. The center is given by m and the diagonal matrix ξ describes the width of the bell in unit directions. We identify a scalar value for ξ with ξI, where I denotes the identity matrix. The parameter c is the number of the component in which the vector field f is non-zero. On the left and right boundary of Ω we provide 10 equidistantly distributed ansatz functions $f[m_i,\xi_i,c_i](x)$. Here $\xi_i = 1.5/10$ and $\xi_i = 1.0/10$ if m_i is located on bottom or top. We always choose c_i such that the ansatz function is tangential to Ω.

We set $\alpha = 1e-10$ and $\epsilon = 0.04$ and stop the optimization as soon as $\|\nabla J(u)\|_U$ is decreased by a factor of 0.1.

In Figure 1 we present the initial phase field φ_0, the desired phse field φ_d and the control areas together with the zero-level lines of φ_0 and φ_d.

The steepest descent method is able to reduce $\|\nabla J\|_U$ from $6e-2$ to $4.6e-2$ in 67 iterations and stagnates due to no further decrease in $\|\nabla J\|_U$. Mean while the functional J is reduced from 0.509 to 0.033. In Figure 2 we show the evolution of φ for the optimal control together with the magnitude of the velocity field.

In Figure 3 we show the evolution of the control action over time. We observe a rapid decay of the control strength at the end of the time horizon, while the first peak corresponds to a strong control at the side walls in the region above the bubble, that is rather inactive after this initial stage.

6.3. Reconstruction of the initial value

Finally we investigate an example of finding an initial phase field, such that after a given amount of time without further control action a desired phase field is achieved. Here we apply only initial value control, i.e. $\alpha_V = \alpha_B = 0$, and we use no-slip boundary conditions for the velocity field.

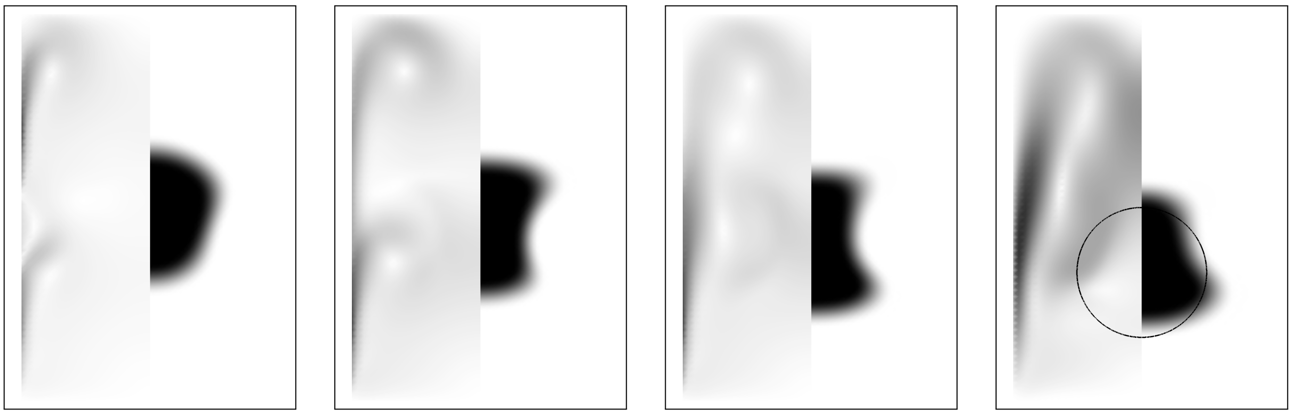

FIGURE 2. The evolution of the optimally controlled phase field and velocity field at times $t = 0.25, 0.5, 0.75, 1.0$ (left to right) when control is only applied to the side walls and not at the bottom and the top part of the boundary. The pictures show the magnitude of the velocity field on the left and the phase field on the right. For $t = 0.1$ we additionally indicate the zero-level line of φ_d by a black line. Note that the velocity field coincides with $B_B u_B$ on the boundary.

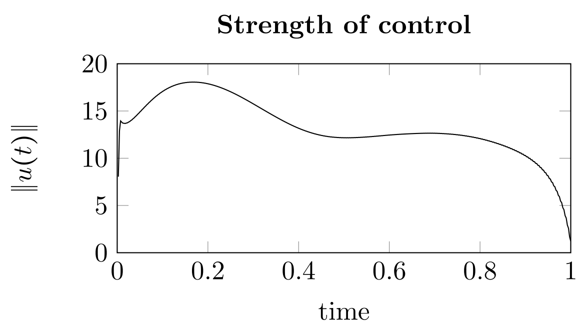

FIGURE 3. The evolution of the optimal control action over time, i.e. $\|u(t)\|$ for the rising bubble example.

Let us turn to the representation of u_I. We initialize u_I with a constant value $u_I = -0.8$ and use a homogeneously refined initial mesh for its representation. We use this mesh for $\mathcal{T}_1$.

After each step of the minimization algorithm we use the jumps accross edges in normal direction of ∇u_I to construct a new grid for the representation of u_I and interpolate the current control to the new grid. The marking is evaluated based on a Dörfler approach.

The parameter for this example are given as $\rho_1 = 1000$, $\rho_2 = 1$, $\eta_1 = 10$, $\eta_2 = 0.1$, $\sigma = 1.245$ and $g \equiv -0.981$. These are the parameters of the second benchmark from [42], where σ was rescaled due to our specific choice of energy. We note that due to the large ratio in density, the bubble undergoes strong deformation during rising. The optimization horizon again is $I = [0, 1.5]$, and $\Omega = (0, 1)^2$. We set $\alpha = 0.2$ and solve the optimization problem for $\epsilon = 0.02$.

We initialize the optimization with $u_I \equiv -0.8$ and use a circle around $M = (0.5, 0.6)$ with radius $r = 0.1763040551$ as defined in (56) as desired shape. These values are used such that $\int_\Omega \varphi_d - u_I \, dx = 0$ is fulfilled.

The optimization problem is solved using the VMPT method, proposed in [15]. It is an extension of the projected gradient method to the Banach space setting. In our situation this is $H^1(\Omega) \cap L^\infty(\Omega)$.

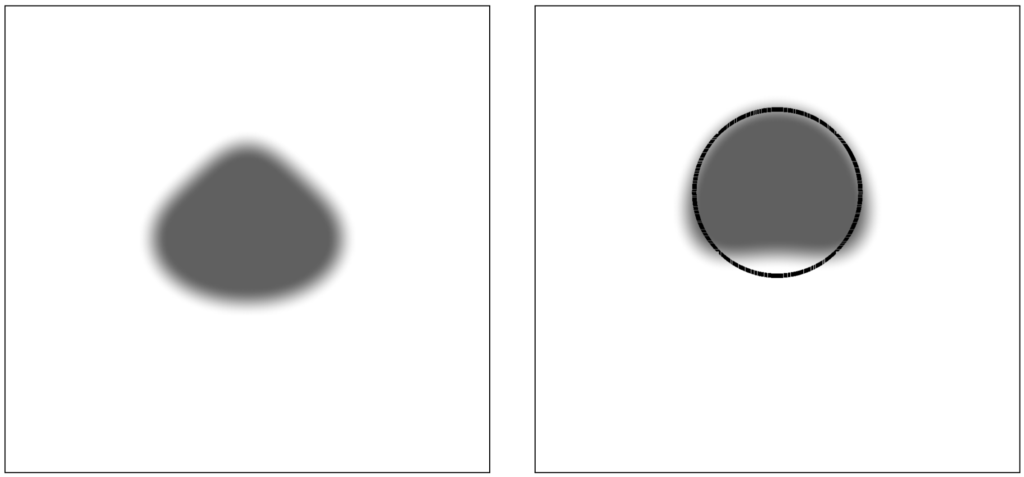

Figure 4. The optimal control u_I (left) and the resulting distribution at the end of the time interval (right), where the bubble is shown in gray. The black line indicates the zero level line of the desired shape.

We stop the allover algorithm as soon as $|(DJ_{u_I}(\cdot), v)| < 1e-3$, where v denotes the current normalized search direction. In our example this is reached after 31 iterations, where J is reduced from 3.8e-1 to 1.9e-1, and especially $\|\varphi^K - \varphi_d\|$ is reduced from 0.43 to 0.16.

In Figure 4 we show the initial shape at the end of the optimization process, on the left and the corresponding shape at the end of the optimization time interval together with the zero level line of the desired shape on the right.

Remark 6.1. In first tests we used an energy for W_u that fulfills Assumptions (A1)–(A5) and the method of steepest descent to solve the resulting optimization problem. There we only got very slow convergence of the algorithm and the resulting optimal u_I had much broader interfaces. So it seems that it is recommended to use the non-smooth free energy as we propose here.

References

[1] GSL - GNU Scientific Library, v1.16. http://www.gnu.org/software/gsl/, 2013.

[2] H. Abels and D. Breit. Weak Solutions for a Non-Newtonian Diffuse Interface Model with Different Densities. *Nonlinearity*, 29:3426–3453, 2016.

[3] H. Abels, D. Depner, and H. Garcke. Existence of weak solutions for a diffuse interface model for two-phase flows of incompressible fluids with different densities. *Journal of Mathematical Fluid Mechanics*, 15(3):453–480, September 2013.

[4] H. Abels, D. Depner, and H. Garcke. On an incompressible Navier–Stokes / Cahn–Hilliard system with degenerate mobility. *Annales de l'Institut Henri Poincaré (C) Non Linear Analysis*, 30(6):1175–1190, 2013.

[5] H. Abels, H. Garcke, and G. Grün. Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Mathematical Models and Methods in Applied Sciences*, 22(3):1150013(40), March 2012.

[6] R. A. Adams and J. H. F. Fournier. *Sobolev Spaces, second edition*, volume 140 of *Pure and Applied Mathematics*. Elsevier, 2003.

[7] S. Aland. Time integration for diffuse interface models for two-phase flow. *Journal of Computational Physics*, 262:58–71, April 2014.

[8] H.W. Alt. *Linear Functional Analysis*. Springer, 2016.

[9] P.R. Amestoy, I.S. Duff, J. Koster, and J.-Y. L'Excellent. A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM Journal of Matrix Analysis and Applications*, 23(1):15–41, 2001.

[10] S. Balay, S. Abhyankar, M.F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, K. Rupp, B.F. Smith, S. Zampini, and H. Zhang. PETSc Web page. http://www.mcs.anl.gov/petsc, 2014.

[11] J.W. Barrett, H. Garcke, and R. Nürnberg. Finite Element Approximation of a Phase Field Model for Surface Diffusion of Voids in a Stressed Solid. *Mathematics of Computation*, 75(253):7–41, 2005.

[12] L. Baňas, M. Klein, and A. Prohl. Control of interface evolution in multiphase fluid flows. *SIAM Journal on Control and Optimization*, 52(4):2284–2318, 2014.

[13] Martin Berggren. Numerical solution of a flow-control problem: Vorticity reduction by dynamic boundary action. *SIAM Journal on Scientific Computing*, 19(3):829–860, 1998.

[14] T. R. Bewley, P. Moin, and R. Temam. DNS-based predictive control of turbulence: an optimal benchmark for feedback algorithms. *Journal of Fluid Mechanics*, 447:179–225, November 2001.

[15] L. Blank and C. Rupprecht. An extension of the projected gradient method to a banach space setting with application in structural topology optimization. *SIAM Journal on Control and Optimization*, 55(3):1481–1499, 2017.

[16] J. F. Blowey and C. M. Elliott. The Cahn–Hilliard gradient theory for phase separation with non-smooth free energy. Part I: Mathematical analysis. *European Journal of Applied Mathematics*, 2:233–280, 1991.

[17] S. C. Brenner and L. R. Scott. *The Mathematical Theory of Finite Element Methods*, volume 15 of *Texts in Applied Mathematics*. Springer, 2008.

[18] C. Carstensen and R. Verfürth. Edge Residuals Dominate A Posteriori Error Estimates for Low Order Finite Element Methods. *SIAM Journal on Numerical Analysis*, 36(5):1571–1587, 1999.

[19] K. Chrysafinos. Stability Estimates of Discontinuous Galerkin Time-Stepping Schemes for the Allen–Cahn Equation and Applications to Optimal Control. *arXiv:1610.05071*, 2016.

[20] W. Dörfler. A convergent adaptive algorithm for Poisson's equation. *SIAM Journal on Numerical Analysis*, 33(3):1106–1124, 1996.

[21] X. Feng and A. Prohl. Numerical analysis of the Allen-Cahn equation and approcimation for mean curvature flows. *Numerische Mathematik*, (94):33–65, 2003.

[22] A.V. Fursikov, M.D. Gunzburger, and L.S. Hou. Boundary Value Problems and Optimal Boundary Control for the Navier–Stokes System: the Two-Dimensional Case. *SIAM Journal on Control and Optimization*, 36(3):852–894, 1998.

[23] H. Garcke, M. Hinze, and C. Kahle. A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow. *Applied Numerical Mathematics*, 99:151–171, January 2016.

[24] J. Geng and Z. Shen. The Neumann problem and Helmholtz decomposition in convex domains. *Journal of Functional Analysis*, 259:2147–2164, 2010.

[25] V. Girault and P. A. Raviart. *Finite Element Methods for Navier–Stokes Equations*, volume 5 of *Springer series in computational mathematics*. Springer, 1986.

[26] G. Grün. On convergent schemes for diffuse interface models for two-phase flow of incompressible fluids with general mass densities. *SIAM Journal on Numerical Analysis*, 51(6):3036–3061, 2013.

[27] G. Grün, F. Guillén-Gonzáles, and S. Metzger. On Fully Decoupled Convergent Schemes for Diffuse Interface Models for Two-Phase Flow with General Mass Densities. *Communications in Computational Physics*, 19(5):1473–1502, May 2016.

[28] G. Grün and F. Klingbeil. Two-phase flow with mass density contrast: Stable schemes for a thermodynamic consistent and frame indifferent diffuse interface model. *Journal of Computational Physics*, 257(A):708–725, January 2014.

[29] F. Guillén-Gonzáles and G. Tierra. Splitting schemes for a Navier–Stokes–Cahn–Hilliard model for two fluids with different densities. *Journal of Computational Mathematics*, 32(6):643–664, 2014.

[30] M.D. Gunzburger and S. Maservisi. The Velocity Tracking Problem for Navier–Stokes Flows With Boundary Control. *SIAM J. Control Optim.*, 39(2):594–634, 2000.

[31] Z. Guo, P. Lin, and J. S. Lowengrub. A numerical method for the quasi-incompressible Cahn–Hilliard–Navier–Stokes equations for variable density flows with a discrete energy law. *Journal of Computational Physics*, 276:486–507, November 2014.

[32] M. Hintermüller, M. Hinze, C. Kahle, and T. Keil. A goal-oriented dual-weighted adaptive finite element approach for the optimal control of a nonsmooth Cahn–Hilliard–Navier–Stokes system. *Hamburger Beiträge zur angewandten Mathematik 2016-25*, 2016.

[33] M. Hintermüller, M. Hinze, and M. H. Tber. An adaptive finite element Moreau–Yosida-based solver for a non-smooth Cahn–Hilliard problem. *Optimization Methods and Software*, 25(4-5):777–811, 2011.

[34] M. Hintermüller, T. Keil, and D. Wegner. Optimal Control of a Semidiscrete Cahn–Hilliard–Navier–Stokes System with Nonmatched Fluid Densities. *SIAM Journal on Control and Optimization*, 55(3):1954–1989, 2017.

[35] M. Hintermüller and D. Wegner. Distributed Optimal Control of the Cahn–Hilliard System Including the Case of a Double-Obstacle Homogeneous Free Energy Density. *SIAM J. Control Optim.*, 50(1):388–418, 2012.

[36] M. Hintermüller and D. Wegner. Optimal Control of a semidiscrete Cahn–Hilliard Navier–Stokes system. *SIAM Journal on Control and Optimization*, 52(1):747–772, 2014.

[37] M. Hinze. Instantaneous closed loop control of the Navier–Stokes system. *SIAM Journal on Control and Optimization*, 44(2):564–583, 2005.

[38] M. Hinze. A variational discretization concept in control constrained optimization: the linear quadratic case. *Computational Optimization and Applications*, 30(1):45–61, 2005.

[39] M. Hinze and C. Kahle. Model Predictive Control of Variable Density Multiphase Flows Governed by Diffuse Interface Models. In *Proceedings of the first IFAC Workshop on Control of Systems Modeled by Partial Differential Equations*, volume 1, pages 127–132, 2013.

[40] M. Hinze and K. Kunisch. Second order methods for boundary control of the instationary Navier-Stokes system. *Zeitschrift für Angewandte Mathematik und Mechanik*, 84(3):171–187, 2004.

[41] M. Hinze, R. Pinnau, M. Ulbrich, and S. Ulbrich. *Optimization with PDE constraints*, volume 23 of *Mathematical Modelling: Theory and Applications*. Springer, 2009.

[42] S. Hysing, S. Turek, D. Kuzmin, N. Parolini, E. Burman, S. Ganesan, and L. Tobiska. Quantitative benchmark computations of two-dimensional bubble dynamics. *International Journal for Numerical Methods in Fluids*, 60(11):1259–1288, 2009.

[43] C. Kahle. Instantaneous control of two-phase flow with different densities. *Oberwolfach Reports, Chapter: Interfaces and Free Boundaries: Analysis, Control and Simulation*, 10(1):898–901, 2013.

[44] C. Kahle. *Simulation and Control of Two-Phase Flow Using Diffuse-Interface Models*. PhD thesis, University of Hamburg, 2014.

[45] C. Kahle. An L^∞ bound for the Cahn–Hilliard equation with relaxed non-smooth free energy density. *International Journal of Numerical Analysis and Modeling*, 14(2):243–254, 2017.

[46] D. Kay, V. Styles, and R. Welford. Finite element approximation of a Cahn–Hilliard–Navier–Stokes system. *Interfaces and Free Boundaries*, 10(1):15–43, 2008.

[47] A. Logg, K.-A. Mardal, and G. Wells, editors. *Automated Solution of Differential Equations by the Finite Element Method - The FEniCS Book*, volume 84 of *Lecture Notes in Computational Science and Engineering*. Springer, 2012.

[48] R. Nürnberg and E.J.W. Tucker. Finite Element Approximation of a Phase Field Model Arising in Nanostructure Patterning. *Numerical Methods for Partial Differential Equations*, 31:1890–1924, 2015.

[49] Y. Oono and S. Puri. Study of phase-separation dynamics by use of cell dynamical systems. I. Modeling. *Physical Review A*, 38(1):434–463, 1988.

[50] A. Schmidt and K. G. Siebert. *Design of adaptive finite element software: The finite element toolbox ALBERTA*, volume 42 of *Lecture Notes in Computational Science and Engineering*. Springer, 2005.

[51] R. Temam. *Navier–Stokes equations - Theory and numerical analysis*. North-Holland Publishing Company, Amsterdam, New York, Oxford, 1977.