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Optimization with Allen-Cahn variational inequalities

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ABSTRACT. Optimization problems governed by Allen-Cahn systems including elastic effects are formulated and first-order necessary optimality conditions are presented. Smooth as well as obstacle potentials are considered, where the latter leads to phase field MPECs.

1. Introduction

The popularity of phase field models have increased in the last two decades in various fields of applied mathematics, physics and engineering sciences. Some examples for their applications are Phase transformations (Solidification of pure substances, solid-solid transformation (i.e. transitions of solids from one crystalline modification to another), melting, freezing, sublimation, evaporation, condensation), Crack growth (as continuum damage), Dislocation dynamics, Multi-phase fluid flows, Topology optimization, Mathematical finance (american option pricing) and Mathematical modelling of biological processes such as cancer growth, wound healing, biofilms, granulomas, blood cells, but its is almost impossible to give a comprehensive and complete list of topics treated with the help of phase field methods, since there is continuous developement of phase field models for new application fields and this is still ongoing reasearch, see [**48**] and references therein. With the help of phase field models the geometry of free boundaries (interfaces) is described through one or several order parameters which are called *phase fields.* Within each separate phase the order parameter doesn't vary and is constant, but one expects large spatial variations of the order parameter across interfaces between different phases. However, the advantage of the phase field models lies in the formulation of the interfaces which are assumed to be diffuse or blurred. The phase boundaries consist of small trasition layers of finite but positive thickness. Hence, explicit front tracking is

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avoided by using smooth continuous phase field variables locating the grain and phase boundaries. By asymptotic expansions for vanishing interface thickness, it can be shown that classical sharp interface models including physical laws at interfaces and multiple junctions are recovered, see [**17**].

The essential ingredients of a phase field model will be symmerized in the following. We note here that we are going to discuss only isothermal phase field models. To this end, the temperatur of our corresponding system will be fixed to a constant temperatur and hence will not appear anywhere in our equations.

Now the first step in our derivation of a phenomenological theory of phase transitions is the definition of a phase field variable (with N different phases) which is described by $\boldsymbol{c} = (c_1, \ldots, c_N)^T$, where c_i (as a scalar quantity) denotes the fraction of the i-th material (In this work we denote vectors by boldface letters). The second step is to consider the non-convex (interfacial) Ginzburg-Landau energy, see [**16**],

$$E(\boldsymbol{c}) := \int_\Omega \left\{ \frac{\varepsilon}{2}|\nabla \mathbf{c}|^2 + \frac{1}{\varepsilon}\Psi(\mathbf{c}) \right\} \, \mathrm{d}x, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, is a bounded domain with either convex or $C^{1,1}$-boundary $\Gamma := \partial\Omega$, the small parameter $\varepsilon > 0$ is related to the interface thickness and Ψ is the bulk potential. In general the potential Ψ is assumed to have global minima at the pure phases and in physical situations there are many choices possible, see [**13**]. Here we distinguish between the choice of a smooth polynomial and a non-smooth obstacle potential. The latter ensures, in particular, that the pure phases correspond exactly to $y_i = 1$, whereas in the smooth case those are given by $y_i \approx 1$.

For the appearance of mechanical effect in the system we additionally consider the energy term $W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u}))$ to the Ginzburg-Landau energy (1.1) which represents the elastic free energy density, see [**29**]. Since in phase separation processes of alloys the deformations are typically small we choose a theory based on the linearized strain tensor (see [**19**]) given by $\mathcal{E} := \mathcal{E}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ and

$$W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) = \frac{1}{2}(\mathcal{E} - \mathcal{E}^*(\boldsymbol{c})) : \mathcal{C}(\mathcal{E} - \mathcal{E}^*(\boldsymbol{c})). \tag{1.2}$$

Here $\mathcal{C}$ is the symmetric, positive definite, possibly anisotropic elasticity tensor mapping from symmetric tensors in $\mathbb{R}^{d\times d}$ into itself. The quantity $\mathcal{E}^*(\boldsymbol{c})$ is the eigenstrain at concentration $\boldsymbol{c}$ and following Vegard's law we choose $\mathcal{E}^*(\boldsymbol{c}) = \sum_{i=1}^N y_i \mathcal{E}^*(\boldsymbol{e}_i)$, where $\mathcal{E}^*(\boldsymbol{e}_i)$ is the value of the strain tensor when the material consists only of component i and is unstressed. Here $(\boldsymbol{e}_i)_{i=1}^N$ denote the standard coordinate vectors in $\mathbb{R}^N$.

Further, other energy contributions can be added without any specific restrictions to the usual Ginzburg-Landau energy (1.1) to take into account additional fields. For example, one can also take into account boundary effects and contributions which are given by additional boundary energies, see [**30**].

Hence, the total free energy of the underlying system consists of all free energies belonging to the corresponding field variable which are take into account for the specific desired modeling by the scientists. Here, we have

$$E_{tot} := E + W, \tag{1.3}$$

Now, we are in a position to determine the equations of state or loosely speaking the dynamics of the interface motion. For the derivation of such an equation it is important whether the order parameter (phase field) of the underlying physical system itself obseys a consevation law or not. We distinguish here the following cases: If the phase field variable represents a density or concentration of some substance, then it follows from the principle of conservation of matter that the dynamical process cannot change the total amount of this substance in the system (provided that there is mass flux over the boundary); it moves parts of the substance from one place to another. In such case, one speaks of a conserved order parameter. Such systems often lead to fourth-order equations of Cahn-Hilliard type, see [**16**] and references therin. However, if the order parameter is, for example, the magnetization in a ferromagnet, then there is no such restriction, and we may speak of a non-conserved order parameter. The latter case is referred to as second-order equations of Allen-Cahn type. In this paper we will only consider the Allen-Cahn type systems.

Allen-Cahn type equations as L^2-Gradient flows. Any Allen-Cahn type equation can be modelled by the steepest descent of (1.3) with respect to the L^2-norm, see [**12, 28**]. The simplest Allen-Cahn eqution is derived if we only consider $E_{tot} := E$ and neglect the mechanical effects ($W = 0$) of the underlying system. The next stage of the generalization of the Allen-Cahn equation is to take into account other fields such as for instance mechanical, boundary effects or other fields. Here, for the Allen-Cahn type equations, we are interested furthermore in two cases: simple Allen-Cahn equations and elastic Allen-Cahn equations. Furthermore, these two cases are considered with smooth potential as well as non-smooth obstacle potentials.

In the following we derive, as an example, the elastic Allen-Cahn equation with no flux boundary condition and non-smooth obstacle potential. Here, it is important to note that the mechanical equilibrium is obtained on a much faster time scale and therefore we assume quasi-static equilibrium for the mechanical variable $\boldsymbol{u}$. For multi-material phase field models the phase space for the order parameter $\boldsymbol{c}$ is given by the Gibbs simplex

$$\boldsymbol{G} := \{\boldsymbol{v} \in \mathbb{R}^N : \boldsymbol{v} \geq \boldsymbol{0}, \boldsymbol{v} \cdot \boldsymbol{1} = 1\}. \tag{1.4}$$

Note that we use the notation $\boldsymbol{v} \geq \boldsymbol{0}$ for $v_i \geq 0$ for all $i \in \{1, \dots, N\}$, $\boldsymbol{1} = (1, \dots, 1)^T$. As indicated for the bulk potential $\Psi : \mathbb{R}^N \to \mathbb{R} \cup \{\infty\}$ we consider the multi-obstacle potential

$$\Psi(\boldsymbol{v}) := \Psi_0(\boldsymbol{v}) + I_G(\boldsymbol{v}) = \begin{cases} \Psi_0(\boldsymbol{v}) := -\frac{1}{2}\|\boldsymbol{v}\|^2 & \text{for } \boldsymbol{v} \in G, \\ \infty & \text{otherwise}, \end{cases} \tag{1.5}$$

where I_G is the indicator function of the Gibbs simplex G. The L^2-steepest descent of the energy $E_{tot} := E + W$ results after suitable rescaling of time in the following elastic Allen-Cahn equation

(1.6)

$$\begin{pmatrix} \varepsilon\partial_t \boldsymbol{c} \\ \boldsymbol{0} \end{pmatrix} = -\mathrm{grad}_{L^2} E(\boldsymbol{c}, \boldsymbol{u}) = \begin{pmatrix} \varepsilon\Delta\boldsymbol{c} + \frac{1}{\varepsilon}(\boldsymbol{c} + \boldsymbol{\xi}) - D_c W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) \\ \nabla \cdot D_{\mathcal{E}} W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) \end{pmatrix},$$

where $-\boldsymbol{\xi} \in \partial I_G$ and ∂I_G denotes the subdifferential of I_G. Moreover, D_c and $D_{\mathcal{E}}$ denote the differentials with respect to $\boldsymbol{c}$ and $\mathcal{E}$, respectively. We have

$$D_c W(\boldsymbol{c}, \mathcal{E}) = -\mathcal{E}^* : \mathcal{C}(\mathcal{E} - \mathcal{E}^*(\boldsymbol{c})) \text{ and } D_{\mathcal{E}} W(\boldsymbol{c}, \mathcal{E}) = \mathcal{C}(\mathcal{E} - \mathcal{E}^*(\boldsymbol{c})). \tag{1.7}$$

Note that, in the case of a nonsmooth obstacle potential, Ψ is given as the sum of a differentiable and a non-differentiable convex function and the derivative $D\Psi(\boldsymbol{c})$ has to be understood as sum of the differentiable part plus the subdifferential of the non-differentiable convex summand, and so the first component of (1.6) is in fact an inclusion. This inclusion can be rewritten both in a variational inequality or in a complementarity formulation, see Section 2.1.2.

REMARK 1.1. In a system with two phases, i.e. $N = 2$, the problem can be reduced to a single unkown by defining $c := c_1 - c_2$, which results in a scalar problem. Further, note that the Gibbs simplex is just the intervall $[-1, 1]$.

1.1. Optimization problems governed by Allen-Cahn systems. The mathematical research literature on optimization problems for phase field systems is scarce. But, this topic is important concerning their huge potential in applications. In the following we give examples, where control problems for phase field systems are of great practical relevenace: In chemical engineering there is a huge interest in the study of the production of relevant crystals with described shapes. For example, engineers would like to control the production of shapes for Barium sulfate, which is an important substance for the production of pharmaceuticals, see [**15, 22**]. Also in many other areas, like materials science, the optimal control of the solidification process towards a target-shape is desired.

In the following we discuss, as a prototypical example, the optimization problem for the elastic Allen-Cahn equation. We establish the ingredients for the formulation of the overall optimization problem and sensibilize the reader about control and state contraints. In preparation of the optimization problem we assume now that a volume force $\boldsymbol{f}$ acts on $\Omega_T := \Omega \times (0, T)$ and a surface load $\boldsymbol{g} \in L^2(0, T; L^2(\Gamma_g, \mathbb{R}^d))$ acts on $\Gamma_g \subset \Gamma := \partial\Omega$ until a given time $T > 0$. Then, with $\Gamma_D := \Gamma \setminus \Gamma_g$, $\Gamma_T := \Gamma \times (0,T)$ and the outer unit normal $\boldsymbol{n}$, the elastic Allen-Cahn system is given by the mechanical system

$$(1.8) \qquad \begin{cases} -\nabla \cdot D_{\mathcal{E}} W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) &= \boldsymbol{0} \quad \text{in } \Omega, \\ \boldsymbol{u} &= \boldsymbol{0} \quad \text{on } \Gamma_D, \\ D_{\mathcal{E}} W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) \cdot \boldsymbol{n} &= \boldsymbol{g} \quad \text{on } \Gamma_g \end{cases}$$

which has to hold for a.e. $t \in (0,T)$, and the Allen-Cahn system

$$(1.9) \qquad \begin{cases} \varepsilon \partial_t \boldsymbol{c} - \varepsilon \Delta \boldsymbol{c} + \frac{1}{\varepsilon} D\Psi(\boldsymbol{c}) + D_{\boldsymbol{c}} W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u})) &= \boldsymbol{f} \quad \text{in } \Omega_T, \\ \nabla \boldsymbol{c} \cdot \boldsymbol{n} &= \boldsymbol{0} \quad \text{on } \Gamma_T, \\ \boldsymbol{c}(0) &= \boldsymbol{c}_0 \quad \text{in } \Omega, \end{cases}$$

where Ψ is not specified yet. For a non-smooth potential the eqution in (1.9) is indeed an inclusion.

Now the optimal control problem with the elastic Allen-Cahn equation consists of the following objective: We want to transform a given initial phase distribution $\boldsymbol{y}_0 : \Omega \to \mathbb{R}^N$ with minimal cost of the controls to some desired phase pattern $\boldsymbol{y}_T \in \boldsymbol{L}^2(\Omega) := L^2(\Omega, \mathbb{R}^N)$ at a given final time $T > 0$ while tracking a desired evolution $\boldsymbol{y}_d \in \boldsymbol{L}^2(\Omega_T) := L^2(0,T; \boldsymbol{L}^2(\Omega))$. Hence, the following tracking-type functional fulfills this requirement:

$$(1.10) \qquad \begin{aligned} J(\boldsymbol{c}, \boldsymbol{f}, \boldsymbol{g}) :=& \frac{\nu_T}{2} \|\boldsymbol{c}(T,\cdot) - \boldsymbol{c}_T\|^2_{\boldsymbol{L}^2(\Omega)} + \frac{\nu_d}{2} \|\boldsymbol{c} - \boldsymbol{c}_d\|^2_{\boldsymbol{L}^2(\Omega_T)} + \\ &+ \frac{\nu_f}{2\varepsilon} \|\boldsymbol{f}\|^2_{\boldsymbol{L}^2(\Omega_T)} + \frac{\nu_g}{2} \|\boldsymbol{g}\|^2_{L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))}. \end{aligned}$$

This leads, in case of a smooth potential Ψ, to the following optimal control problem:

$$(1.11) \qquad (\mathcal{P}) \begin{cases} \text{min} & J(\boldsymbol{c}, \boldsymbol{f}, \boldsymbol{g}) \\ \text{over} & (\boldsymbol{c}, \boldsymbol{f}, \boldsymbol{g}) \in \boldsymbol{\mathcal{V}} \times \boldsymbol{L}^2(\Omega_T) \times L^2(0,T; L^2(\Gamma_g, \mathbb{R}^d)) \\ \text{s.t.} & (1.8) \text{ and } (1.9) \text{ hold} \end{cases}$$

with $\boldsymbol{\mathcal{V}} := L^\infty(0,T; \boldsymbol{H}^1(\Omega)) \cap H^1(0,T; \boldsymbol{L}^2(\Omega)) \cap L^2(0,T; \boldsymbol{H}^2(\Omega))$. We assume, that the Dirichlet part Γ_D has positive $(d-1)$-dimensional Hausdorff measure and introduce the notation $H^1_D(\Omega, \mathbb{R}^d) := \{\boldsymbol{u} \in H^1(\Omega, \mathbb{R}^d) \mid \boldsymbol{u}|_{\Gamma_D} = \boldsymbol{0}\}$. Later on we will use also the space $\boldsymbol{\mathcal{W}}(0,T) := L^2(0,T; \boldsymbol{H}^1(\Omega)) \cap H^1(0,T; \boldsymbol{H}^1(\Omega)^*)$.

By virtue of pratical considerations and limitations of control resources, people usually take into account control contraints, i.e. the control is confined into a given admissible set. More precisely, in most cases, admissible control sets are convex and closed and don't cause additional mathematical difficulties. Things get more delicate, if state contraints enter the optimization problem and this is the case if we consider the non-smooth obstacle potential (1.5). As indicated before, in (1.9) we obtain then an inclusion which stems from the subdifferential of the indicator function of the Gibbs-simplex (the subdifferential contains implicitly the state constraint). Therefore state constraints appear in a direct natural way in optimization problems with phase field equations, and they lead to optimization problems with phase field variational inequalities which can be interpreted as MPECs in function spaces.

General MPECs. In the field of mathematical programs with equilibrium constraints (MPECs) one is faced with a constraint optimization problems, where the decision/state variables satisfy a variational inequality and hence often model equilibrium systems. These systems can, therefore, be interpreted as optimization problems themselves, and are considered as generalizations of so-called bilevel (or multilevel) optimization problems. Due to the variational inequality structure of the contraint in MPECs standard constraints qualifications of classical optimization theory such as the linear independenece (LICQ) or Mangasarian-Fromovitz constraint qualifications (MFCQ) are generally violated. Hence, alternative strategies have to be developed and employed in order to derive optimality conditions. To this end, there has been a considerable amount of attention in the past in the finite-dimensional MPECs, and a whole hierachy of stationarity concepts for these finite-dimensional MPECs have been developed, including the notions of *weak-*, *C(lark)-*, *M(ordukovich)-*, and *strong stationarity*; see, e.g. [**49**]. For the MPECs formulated in infinite dimensional function spaces, however, the topic is still in its infancy and there exists less research. A state-of-the-art overview of the works and mathematical literature up to the 1980 can be found in [**1**]. Since then, there has been a number of research efforts and the mathematical literature has increased; see e.g., the works in [**3, 4, 5, 6, 9, 26, 27, 34, 42, 45, 46**]. But still, the overall research level is far less complete when compared to finite diemensions and, as far as stationarity principles are concerned, significantly less complete and systematic. This makes MPECs especially challenging from mathematical point of view. In function space setting, in principle, the above mentioned finite-dimensional stationarity concepts are available as well. However, depending on certain conditions and specific to the function space context as the realization of the variational inequality-constraint and the induced regularity of the associated Lagrange multipliers, it turns out that there exist finer classifications of stationarity notions, such as weak C-stationarity or even weaker, which stem from the possible ambiguity of pointwise condition that arise in our function space setting and are all equivalent in finite dimensions. We refer to [**43**] for a comprehensive classification of stationarity concepts for MPECs in infinite dimensional function spaces.

Particular instances for MPECs in functions spaces are optimization problems with partial differential inequalities (or inclusions). Many authors, i.e. see [**1, 46, 14, 26, 27, 9, 4, 8, 7, 32, 31, 18, 47**], have already considered control problems for many elliptic and some parabolic variational inequalities and different mathematical techniques have been applied and developed to tackle and solve these problems. In [**1, 2**], approximations (penalizations) of the variational inequality which lead to optimal control problems governed by variational equations are studied and existence results and optimality conditions using a passage to the limit in the approximation process are derived. Other authors have considered in many different scenarios venues aspects, for example regularization-relaxation [**4**], Pontryagin's principle [**8, 14**], Ekeland's principle with diffuse perturbations [**8**], conical derivatives [**46**] and refernces therein. Especially for the numerical treatment of MPECs, we refer to [**40, 41, 35, 36**]. These recent works have in common that they apply mathematical methods and proof-steps, which highly motivate efficient numerical algorithms.

Phase field MPECs. Optimal control problems with phase field variational inequalities are particular instances of infinite dimensional MPECs. To the best of our knowledge, the paper [**24**] is the first work discussing an Allen-Cahn MPEC. Since then the papers [**23, 25, 10, 21, 20, 38, 39, 50**] appeared and represent futher attempts in this direction. The general strategy, in all of these works, consists in exploiting an approximation technique to derive optimality systems. Due to the time-dependency of the phase field MPECs the process of the passage to the limit is the most delicate part and requires more sophisticated arguments than the corresponding analysis for the standard elliptic MPECs. The reason lies in the lack of regularity for the corresponding time-dependent dual multiplers. Consequently the adjoint variables posseses weak time-regularity and hence the time-derivative of the adjoint variable converges in a very weak topology. Moreover, C-stationarity of the limit points is only given in the sense of weakly-weakly convergent pairings of the primal and dual multipliers.

The rest of this article is organized as follows. In section 2 we will discuss and summerize the results of the papers [**10, 24, 23, 25**]. The general solution strategy is as following: The primary MPEC will be modified into a "treatable" optimal control problem for which existence of an optimal control and an optimality system of first-order is derived by exploiting optimization theory in Banach spaces. Finally a limit problem is established and interpreted as an optimality system for the original MPEC.

2. Detailed Considerations about Allen-Cahn MPECs

2.1. First-order optimality conditions. In this section we discuss the existence of a minimizer and the derivation of first-order necessary optimality systems. First we present the smooth potential case. Here, the standard optimization theory in function spaces is applicable and delivers a first-order necessary optimality system. Afterwards, we focus on the control problem with an obstacle potential leading to an optimal control problem with variational inequalities. As discussed in the previous section, this belongs to the class of MPECs, where the standard control theory is in general not applicable. Here we employ a penalty approach for the problem without distributed control and a relaxation approach for the model without elasticity.

2.1.1. *Smooth polynomial* Ψ. We start by considering the setting without volume force, i.e. $\boldsymbol{f} \equiv \mathbf{0}$. One typical choice of a smooth potential is then the double-well potential $\Psi(c) = \frac{1}{4}(c^2-1)^2$. The scalar case with this Ψ is studied extensively in [**33**] without tracking c_d, i.e. $\nu_d = 0$. For a regularized obstacle potential Ψ_σ (see Subsection 2.1.3) the vector-valued case with possibly $\nu_d \neq 0$ is discussed in [**25**]. However, Ψ_σ is not a physical potential. The following theorem summarizes the results of [**25, 33**].

THEOREM 2.1. *Let $(\mathcal{P})$ be given as a scalar problem for $N = 2$ with potential $\Psi = \frac{1}{4}\left(c^2-1\right)^2$ and $\nu_d = 0$ or for $N \geq 2$ and $\nu_d \geq 0$ arbitrary with a regularized obstacle potential Ψ_σ as mentioned above. For fixed initial distribution $\boldsymbol{c}_0 \in \boldsymbol{H}^1(\Omega)$ and given surface load $\boldsymbol{g} \in L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))$ there exists a unique solution $(\boldsymbol{c},\boldsymbol{u}) \in \boldsymbol{\mathcal{V}} \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d))$ of* (1.8)-(1.9) *and hence the solution operator $\boldsymbol{S} : L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d)) \to \boldsymbol{\mathcal{V}} \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d))$ with its components $\boldsymbol{S}(\boldsymbol{g}) := (\boldsymbol{S}_1(\boldsymbol{g}),\boldsymbol{S}_2(\boldsymbol{g})) = (\boldsymbol{c},\boldsymbol{u})$ is well-defined.*

Then the control problem $(\mathcal{P})$ is equivalent to minimizing the reduced cost functional $j(\boldsymbol{g}) := J(\boldsymbol{S}_1(\boldsymbol{g}),\boldsymbol{g})$ over $L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))$. This result is established by applying energy methods to a time-discretized version of (1.8)-(1.9) and showing a series of uniform a priori estimates for the time discretized solutions, where one has to consider the particular functions Ψ and Ψ_σ, respectively, and the coupling of the systems. By the direct method in the calculus of variations one can then show existence of a minimizer for $(\mathcal{P})$. The differentiability of the solution operator can be shown by an implicit function argument and thus we can differentiate the reduced cost functional to obtain the following necessary optimality condition:

THEOREM 2.2. *Every minimizer $\boldsymbol{g} \in L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))$ of j fulfills the following optimality system:* (1.8), (1.9) *and*

$$\boldsymbol{q} + \nu_g \boldsymbol{g} = \boldsymbol{0} \quad \text{a.e. on } (0,T)\times\Gamma_g, \tag{2.1}$$

(2.2)
$$\begin{cases} -\varepsilon\partial_t \boldsymbol{p} - \varepsilon\Delta\boldsymbol{p} + \frac{1}{\varepsilon}D^2\Psi(\boldsymbol{c})\boldsymbol{p} + D_{\boldsymbol{p}}W(\boldsymbol{p},\mathcal{E}(\boldsymbol{q}))) &= \nu_d(\boldsymbol{c}-\boldsymbol{c}_d), \quad \text{in } \Omega_T, \\ \nabla\boldsymbol{p}\cdot\boldsymbol{n} &= \boldsymbol{0} \quad \text{on } \Gamma_T, \\ \varepsilon\boldsymbol{p}(T) &= \nu_T(\boldsymbol{c}(T)-\boldsymbol{c}_T) \quad \text{in } \Omega, \end{cases}$$

$$\begin{cases} -\nabla\cdot D_{\mathcal{E}}W(\boldsymbol{p},\mathcal{E}(\boldsymbol{q})) &= \boldsymbol{0} \quad \text{in } \Omega, \\ \boldsymbol{q} &= \boldsymbol{0} \quad \text{on } \Gamma_D, \\ D_{\mathcal{E}}W(\boldsymbol{p},\mathcal{E}(\boldsymbol{q}))\cdot\boldsymbol{n} &= \boldsymbol{0} \quad \text{on } \Gamma_g. \end{cases} \tag{2.3}$$

For a setting without elasticity but with distributed control, i.e. $\boldsymbol{f} \not\equiv \boldsymbol{0}$ and arbitrary $\nu_d, \nu_T \geq 0$, we refer for instance to [**24**]. There, the scalar case, i.e. $N = 2$ as above, is considered with a penalized double obstacle potential Ψ_σ. Moreover, the optimality system is investigated rigorously and is given by (1.9), (2.2) without elastic energy together with the gradient equation

$$\boldsymbol{p} + \frac{\nu_f}{\varepsilon}\boldsymbol{f} = \boldsymbol{0} \quad \text{a.e. in } \Omega_T. \tag{2.4}$$

2.1.2. *Obstacle potential.* In the case of an obstacle potential each component of $\boldsymbol{c}$ stands, in contrast to the smooth potential, exactly for the fraction of one phase. Hence the phase space is the Gibbs simplex (1.4) and the bulk potential $\Psi : \mathbb{R}^N \to \mathbb{R} \cup \{\infty\}$ is the multi-obstacle potential (1.5), which we consider. As discussed before, the differential of the indicator function has to be understood in the sense of subdifferentials, and thus the Allen-Cahn system (1.9) results in a variational inequality, which can also be written in the following form (see [**11**]):

$$
(2.5) \quad \left\{ \begin{array}{rcll} \varepsilon\partial_t \boldsymbol{c} - \varepsilon\Delta \boldsymbol{c} - \boldsymbol{P}_\Sigma \left(\frac{1}{\varepsilon}(\boldsymbol{c}+\boldsymbol{\xi}) - D_c W(\boldsymbol{c}, \mathcal{E}(\boldsymbol{u}))\right) & = & \boldsymbol{f} & \text{in } \Omega_T, \\ \nabla \boldsymbol{c}\cdot \boldsymbol{n} & = & \boldsymbol{0} & \text{on } \Gamma_T, \\ \boldsymbol{c}(0) & = & \boldsymbol{c}_0 & \text{in } \Omega, \end{array} \right.
$$

together with the complementarity conditions

$$
(2.6) \qquad \boldsymbol{c} \geq \boldsymbol{0} \text{ a.e. in } \Omega_T,\ \boldsymbol{\xi} \geq \boldsymbol{0} \text{ a.e. in } \Omega_T,\ (\boldsymbol{\xi}, \boldsymbol{c})_{L^2(\Omega_T)} = 0,
$$

the additional constraint $\boldsymbol{c} \in \boldsymbol{\Sigma} := \{\boldsymbol{v} \in \mathbb{R}^N \mid \sum_{i=1}^N v_i = 1\}$ a.e. in Ω_T and the requirement $\boldsymbol{f} \in \boldsymbol{T\Sigma} := \{\boldsymbol{v} \in \mathbb{R}^N \mid \sum_{i=1}^N v_i = 0\}$ a.e. in Ω_T. Here $\boldsymbol{P}_\Sigma : \mathbb{R}^N \to \boldsymbol{T\Sigma}$ is the projection operator defined by $\boldsymbol{P}_\Sigma \boldsymbol{v} := \boldsymbol{v} - \boldsymbol{1}\frac{1}{N}\sum_{i=1}^{N} v_i$. The variable $\boldsymbol{\xi}$ can be interpreted as a Lagrange multiplier corresponding to the constraint $\boldsymbol{c} \geq \boldsymbol{0}$, and as a slack variable used for reformulating the variational inequality into a standard MPEC problem. Denoting $\boldsymbol{L}^2_{\boldsymbol{T\Sigma}}(\Omega_T) := \{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega_T) \mid \boldsymbol{v} \in \boldsymbol{T\Sigma} \text{ a.e. in } \Omega_T\}$ and $\boldsymbol{\mathcal{V}}_{\boldsymbol{T\Sigma}}$, $\boldsymbol{\mathcal{V}}_{\boldsymbol{\Sigma}}$ respectively, the optimal control problem in the case of the obstacle potential is given by

$$
(2.7) \quad (\mathcal{P}_0) \left\{ \begin{array}{ll} \min & J(\boldsymbol{c}, \boldsymbol{f}, \boldsymbol{g}) \\ \text{over} & (\boldsymbol{c}, \boldsymbol{f}, \boldsymbol{g}) \in \boldsymbol{\mathcal{V}}_{\boldsymbol{\Sigma}} \times \boldsymbol{L}^2_{\boldsymbol{T\Sigma}}(\Omega_T) \times L^2(0,T; L^2(\Gamma_g, \mathbb{R}^d)) \\ \text{s.t.} & (1.8), (2.5) \text{ and } (2.6) \text{ hold.} \end{array} \right.
$$

The optimization problem $(\mathcal{P}_0)$ belongs to the problem class of so-called MPECs (Mathematical Programs with Equilibrium Constraints) which violate classical NLP constraint qualifications. In the next two subsections we present results concerning first-order necessary optimality systems obtained by the penalization approach, see [**25**], or the relaxation approach, see [**23**]. These techniques have been discussed also in [**4, 37, 38**].

2.1.3. *Penalization approach without distributed control.* In this section we discuss the penalization approach for the case $\boldsymbol{f} \equiv \boldsymbol{0}$. Following [**25**] we replace the indicator function for the Gibbs simplex I_G by a convex function $\tilde{\psi}_\sigma \in C^2(\mathbb{R})$, $\sigma \in (0,1]$, given by $\tilde{\psi}_\sigma(r) := 0$ for $r \geq 0$, $\tilde{\psi}_\sigma(r) := -\frac{1}{6\sigma^2}r^3$ for $-\sigma < r < 0$ and $\tilde{\psi}_\sigma(r) := \frac{1}{2\sigma}\left(r + \frac{\sigma}{2}\right)^2 + \frac{\sigma}{24}$ for $r \leq -\sigma$, and define the regularized potential function by $\Psi_\sigma(\boldsymbol{c}) = \Psi_0(\boldsymbol{c}) + \hat{\Psi}(\boldsymbol{c})$ with $\hat{\Psi}(\boldsymbol{c}) := \sum_{i=1}^{N} \tilde{\psi}_\sigma(c_i)$. For the resulting penalized optimal control problem denoted by $(\mathcal{P}_\sigma)$, exploiting techniques as in Section 2.1.1, we derive for $\sigma \in (0,1]$ first-order necessary optimality conditions. Proving a priori estimates, uniformly in $\sigma \in (0,1]$, employing compactness and monotonicity arguments and using the definition $\mathcal{W}_0(0,T) = \{\boldsymbol{v} \in \mathcal{W}(0,T) : \boldsymbol{v}(0,\cdot) = \mathbf{0}\}$ with dual space $\mathcal{W}_0(0,T)^*$, where the dual pairing between elements $\boldsymbol{\zeta} \in \mathcal{W}_0(0,T)^*$ and $\boldsymbol{v} \in \mathcal{W}_0(0,T)$ is denoted by $\langle\langle \boldsymbol{\zeta}, \boldsymbol{v} \rangle\rangle$, we are able to show the following existence and approximation result:

THEOREM 2.3. *Whenever $\{\boldsymbol{g}_\sigma\} \subset L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))$ is a sequence of optimal controls for $(\mathcal{P}_\sigma)$ with the sequence of corresponding states $(\boldsymbol{c}_\sigma, \boldsymbol{u}_\sigma, \boldsymbol{\xi}_\sigma) \in \mathcal{V}_{\boldsymbol{\Sigma}} \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d)) \times \boldsymbol{L}^2(\Omega_T)$, where $-\boldsymbol{\xi}_\sigma := D\hat{\Psi}(\boldsymbol{c}_\sigma)$, and adjoint variables $(\boldsymbol{p}_\sigma, \boldsymbol{q}_\sigma, \boldsymbol{\zeta}_\sigma) \in \mathcal{V}_{\boldsymbol{T\Sigma}} \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d)) \times \boldsymbol{L}^2(\Omega_T)$, where $-\boldsymbol{\zeta}_\sigma := D^2\hat{\Psi}(\boldsymbol{c}_\sigma)\boldsymbol{p}_\sigma$, there exists a subsequence, which is denoted again by $\{\boldsymbol{g}_\sigma\}$, that converges weakly to $\boldsymbol{g}$ in $L^2(0,T;L^2(\Gamma_g,\mathbb{R}^d))$. Moreover, $\boldsymbol{g}$ is an optimal control of $(\mathcal{P}_0)$ with corresponding states $(\boldsymbol{c},\boldsymbol{u},\boldsymbol{\xi}) \in \mathcal{V}_{\boldsymbol{\Sigma}} \times \boldsymbol{L}^2(\Omega_T) \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d))$ and adjoint variables $(\boldsymbol{p},\boldsymbol{q},\boldsymbol{\zeta}) \in L^2(0,T;\boldsymbol{H}^1(\Omega)) \times L^2(0,T;H^1_D(\Omega,\mathbb{R}^d)) \times \mathcal{W}_0(0,T)^*$ and we have for $\sigma \searrow 0$:*

(2.8)

$$\begin{array}{llll}
\boldsymbol{c}_\sigma & \longrightarrow \boldsymbol{c} & \textit{weakly} & \textit{in } H^1(0,T;\boldsymbol{L}^2(\Omega)) \cap L^2(0,T;\boldsymbol{H}^2(\Omega)), \\
\boldsymbol{u}_\sigma & \longrightarrow \boldsymbol{u} & \textit{weakly} & \textit{in } L^2(0,T;H^1_D(\Omega,\mathbb{R}^d)), \\
\boldsymbol{\xi}_\sigma & \longrightarrow \boldsymbol{\xi} & \textit{weakly} & \textit{in } \boldsymbol{L}^2(\Omega_T), \\
\boldsymbol{p}_\sigma & \longrightarrow \boldsymbol{p} & \textit{weakly} & \textit{in } L^2(0,T;\boldsymbol{H}^1(\Omega)), \\
\boldsymbol{q}_\sigma & \longrightarrow \boldsymbol{q} & \textit{weakly} & \textit{in } L^2(0,T;H^1_D(\Omega,\mathbb{R}^d)), \\
\boldsymbol{P}_{\boldsymbol{\Sigma}}(\boldsymbol{\zeta}_\sigma) & \longrightarrow \boldsymbol{\zeta} & \textit{weakly-star} & \textit{in } \mathcal{W}_0(0,T)^*.
\end{array}$$

Furthermore we obtain first order conditions:

THEOREM 2.4. *The following optimality system holds for the limit elements $(\boldsymbol{g},\boldsymbol{c},\boldsymbol{u},\boldsymbol{\xi})$ with adjoint variables $(\boldsymbol{p},\boldsymbol{q},\boldsymbol{\zeta})$ of Theorem 2.3:* (1.8), (2.1), (2.3), (2.5), (2.6), $\boldsymbol{c} \in \boldsymbol{\Sigma}$, $\boldsymbol{f} \in \boldsymbol{T\Sigma}$ *a.e. in* Ω_T *and*

$$\begin{aligned}
&-\frac{1}{\varepsilon}\langle\langle \boldsymbol{\zeta}, \boldsymbol{v} \rangle\rangle + \varepsilon \int_0^T \langle \partial_t \boldsymbol{v}, \boldsymbol{p} \rangle \,\mathrm{d}t + \varepsilon \int_0^T \int_\Omega \nabla \boldsymbol{p} \cdot \nabla \boldsymbol{v} \,\mathrm{d}x\,\mathrm{d}t + \\
&-\frac{1}{\varepsilon}\int_0^T \int_\Omega \boldsymbol{p} \cdot \boldsymbol{v} \,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_\Omega \boldsymbol{P}_{\boldsymbol{\Sigma}}(D_{\boldsymbol{p}} W(\boldsymbol{p}, \mathcal{E}(\boldsymbol{q}))) \cdot \boldsymbol{v} \,\mathrm{d}x\,\mathrm{d}t + \\
&-\int_0^T \int_\Omega \nu_d(\boldsymbol{c} - \boldsymbol{c}_d) \cdot \boldsymbol{v} \,\mathrm{d}x\,\mathrm{d}t - \int_\Omega \nu_T(\boldsymbol{c}(T,\cdot) - \boldsymbol{c}_T) \cdot \boldsymbol{v}(T) \,\mathrm{d}x = 0,
\end{aligned} \tag{2.9}$$

which has to hold for all $v \in \mathcal{W}_0(0,T)$. Moreover, the limit elements satisfy some sort of complementarity slackness conditions:

$$\lim_{\sigma \searrow 0} (\boldsymbol{\zeta}_\sigma, \boldsymbol{p}_\sigma)_{\boldsymbol{L}^2(\Omega_T)} \leq 0, \tag{2.10}$$

$$\lim_{\sigma \searrow 0} (\boldsymbol{\zeta}_\sigma, \max(\boldsymbol{0}, \boldsymbol{c}_\sigma))_{\boldsymbol{L}^2(\Omega_T)} = 0, \tag{2.11}$$

$$\lim_{\sigma \searrow 0} (\boldsymbol{p}_\sigma, \boldsymbol{\xi}_\sigma)_{\boldsymbol{L}^2(\Omega_T)} = 0. \tag{2.12}$$

REMARK 2.5. The scalar Allen-Cahn case with $\boldsymbol{f} \not\equiv \boldsymbol{0}$ but without elasticity is studied by similar techniques as in [**25**] using a penalization approach. Therefore, we skip the details and refer the reader to [**24**].

2.1.4. *Relaxation approach with distributed control and without elasticity.* Studying the control problem with distributed control, i.e. $\boldsymbol{f} \not\equiv \boldsymbol{0}$ in general, and without elasticity we use a relaxation approach. Details for our presented results can be found in [**23**]. After reformulating as in (2.5) – (2.6) the Allen-Cahn system with the help of a slack variable $\boldsymbol{\xi}$ into an MPEC, we add to the problem $(\mathcal{P}_0)$ an additional constraint $\frac{1}{2}\|\boldsymbol{\xi}\|^2_{\boldsymbol{L}^2(\Omega_T)} \leq R$ and denote this modified optimization problem by $(\mathcal{P}_R)$. The constant R is sufficiently large. This approach is also used in [4] where the control of an obstacle problem is considered. As a first step we treat the state constraint $\boldsymbol{c} \geq \boldsymbol{0}$, which usually raises problems concerning regularity, by adding a regularization term to J. I.e. we define $J_\gamma(\boldsymbol{c}, \boldsymbol{f}) = J(\boldsymbol{c}, \boldsymbol{f}) + \frac{1}{2\gamma\varepsilon} \sum_{i=1}^{N} \|\max(0, \overline{\lambda} - \gamma c_i)\|^2_{L^2(\Omega_T)}$ where $\overline{\lambda} \in L^2(\Omega_T)$ is fixed, nonnegative and corresponds to a regular version of the multiplier associated to $\boldsymbol{c} \geq \boldsymbol{0}$. Next we relax the complementarity condition to $(\boldsymbol{\xi}, \boldsymbol{c})_{\boldsymbol{L}^2(\Omega_T)} \leq \varepsilon\alpha_\gamma$ for some $\alpha_\gamma > 0$. We denote this regularized relaxed version of $(\mathcal{P}_R)$ as $(\mathcal{P}_{R,\gamma})$. Subsequently we are interested in $\gamma \nearrow \infty$ where simultaneously $\alpha_\gamma \searrow 0$. We are able to use techniques from mathematical programming in Banach spaces, see [**44**], and get an optimality system for $(\mathcal{P}_{R,\gamma})$, where γ is fixed. Considering $\gamma \nearrow \infty$ we then obtain optimality conditions for problem $(\mathcal{P}_R)$. Similar to the process in Section 2.1.3 we have: for any $\gamma > 0$ there exists a minimizer $(\boldsymbol{c}_\gamma, \boldsymbol{f}_\gamma, \boldsymbol{\xi}_\gamma) \in \boldsymbol{V}_{\boldsymbol{\Sigma}} \times \boldsymbol{L}^2(\Omega_T) \times \boldsymbol{L}^2(\Omega_T)$ of $(\mathcal{P}_{R,\gamma})$ with corresponding adjoint variables. Using the Lagrange multiplier $r_\gamma \in \mathbb{R}$ of the constraint $(\boldsymbol{\xi}_\gamma, \boldsymbol{c}_\gamma)_{\boldsymbol{L}^2(\Omega_T)} \leq \varepsilon\alpha_\gamma$ one defines $\zeta_{\gamma,i} := r_\gamma \xi_{\gamma,i} - \max(0, \overline{\lambda} - \gamma c_{\gamma,i})$ and $\boldsymbol{\zeta}_\gamma := (\zeta_{\gamma,i})_{i=1}^N$. Then we obtain:

THEOREM 2.6. *Whenever $\{\boldsymbol{f}_\gamma\}$ is a sequence of optimal controls for $(\mathcal{P}_{R,\gamma})$ with the sequence of corresponding states $(\boldsymbol{c}_\gamma, \boldsymbol{\xi}_\gamma)$ and adjoint variables $(\boldsymbol{p}_\gamma, \boldsymbol{\zeta}_\gamma)$, there exists a subsequence, which is denoted the same, with $\boldsymbol{f}_\gamma \to \boldsymbol{f}$ weakly in $\boldsymbol{L}^2(\Omega_T)$ and $\boldsymbol{\zeta}_\gamma \to \boldsymbol{\zeta}$ weakly-star in $\mathcal{W}_0(0,T)^*$ as $\gamma \nearrow \infty$. The convergence of the variables $\boldsymbol{c}_\gamma$, $\boldsymbol{\xi}_\gamma$ and $\boldsymbol{p}_\gamma$ is as in* (2.8). *These limits fulfill the corresponding optimality system for $(\mathcal{P}_R)$ as in Theorem 2.4 without elasticity system but with distributed control, i.e.* (2.4), (2.5), (2.6), (2.9), $\boldsymbol{c} \in \boldsymbol{\Sigma}$, $\boldsymbol{f} \in \boldsymbol{T\Sigma}$ *a.e. in* Ω_T *and the limits with* $(\boldsymbol{p}_\gamma, \zeta_\gamma)$ *satisfy the complementarity slackness conditions* (2.10)-(2.12) *for* $\gamma \nearrow \infty$ *instead of* $\sigma \searrow 0$. *In addition we have the constraint* $\frac{1}{2}\|\boldsymbol{\xi}\|^2_{L^2(\Omega_T)} \leq R$.

REMARK 2.7. The last inequality is in practice inactive using R large enough.

REMARK 2.8. The relations (2.10),(2.11), and (2.12) always have to be understood in a limiting sense and in general such a relation will not be fulfilled for the limit elements. This is mainly due to the lack of regularity of the dual variables and the weak converging results. Therefore, the optimality system given by Theorem 2.4 define a weak form of C-stationarity for the Allen-Cahn MPEC $(\mathcal{P}_0)$.

In this treatise we used mathematical methods and proof-steps which highly motivate numerical algorithms. The regularized problems can be used for reliable numerics for the optimization problems with classical or elastic vector-valued Allen-Cahn variational inequalities, because the latter has a complicated non-smooth structure which is not easy to handle numerically. A first step towards numerical simulation using such an approach has been discussed briefly in [**10**].

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