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AN L^∞ BOUND FOR THE CAHN–HILLIARD EQUATION WITH RELAXED NON-SMOOTH FREE ENERGY

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Abstract. Phase field models are widely used to describe multiphase systems. Here a smooth indicator function, called phase field, is used to describe the spatial distribution of the phases under investigation. Material properties like density or viscosity are introduced as given functions of the phase field. These parameters typically have physical bounds to fulfil, e.g. positivity of the density. To guarantee these properties, uniform bounds on the phase field are of interest. In this work we derive a uniform bound on the solution of the Cahn–Hilliard system, where we use the double-obstacle free energy, that is relaxed by Moreau–Yosida relaxation.

Key words. Cahn–Hilliard, Moreau–Yosida relaxation, phase field equations, uniform bounds.

1. Introduction

Phase field models are a common approach to describe fluid systems of two or more components and to deal with the complex topology changes that might appear in such systems. One of the basic models is the Cahn–Hilliard system [7] that models spinodal decomposition of a binary metal alloy with components having essentially the same density. Particles are only transported by diffusion. Based on this model several extensions to transport by convection (model 'H' [19]) and additionally to fluids with different densities are proposed throughout the literature, see [1,6,9,22]. In those models typically the density and viscosity of the two fluid components are introduced as given functions of a phase field that is introduced to describe their spatial distribution and that is the solution of a Cahn–Hilliard type equation. In general for the Cahn–Hilliard equation with smooth free energies, which allow non-physical values of the phase field, no $L^\infty(\Omega)$ bounds are available. As a consequence, in general situations one can not guarantee that the density and the viscosity of the fluids stay positive, i.e. one might run into non-physical data.

On the other hand, having convergence rates and given a desired dependence between phase field and density, e.g. a linear dependence, one might calculate a maximum violation of the bounds on the phase field such that the density stays positive. Based on this and the desired estimates for the $L^\infty(\Omega)$ violation of the bounds on the phase field, one has a guideline for choosing an appropriate value for the Moreau–Yosida parameter. From the view of approximating the non-smooth double-obstacle free energy by a relaxed free energy, this rate also might be used to derive update rules for the relaxation parameter in a path following method.

In this work we summarize, combine and extend results on the analytical treatment of the Cahn–Hilliard equation with double-obstacle free energy, which is relaxed using Moreau–Yosida relaxation. The aim of this work is, to help later work on Cahn–Hilliard type models by providing $L^\infty(\Omega)$ bounds on the violation of the physical meaningful values of the phase field.

Using Moreau–Yosida relaxation for the treatment of the Cahn–Hilliard equation with double-obstacle free energy is first analytically investigated in [14]. Therein

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especially the convergence of the solutions of the relaxed system to the solution of the double-obstacle system is shown. One main ingredient is the interpretation of the Cahn–Hilliard equation as the first order optimality conditions of a suitable optimal control problem with box constraints in $H^1(\Omega)$ on the control.

On the other hand, in [18], a typical optimal control problem with box constraints in $C(\bar{\Omega})$ on the state is investigated. Here the constraints are treated using Moreau–Yosida relaxation. The authors provide decay rates for the $L^\infty(\Omega)$ norm of the violation of the box constraints in terms of the relaxation parameter. The proof relies on higher regularity of the state, i.e. Hölder regularity is used.

The results in [18] apply for the case of Dirichlet boundary data on the state, while in [15] these results are used for the Cahn–Hilliard equation with Neumann boundary data, to prove convergence of solutions for a relaxed equation to the solutions of a Cahn–Hilliard system with double-obstacle free energy. However, in [15] no convergence rate is provided.

Here we combine the aforementioned results to obtain an $L^\infty(\Omega)$ bound on the violation of the physically meaningful values of the solution of the Cahn–Hilliard equation that can later be used in more sophisticated models where bounds on parameters, like the density, that depend on the solution of the Cahn–Hilliard equation, are required.

The paper is organized as follows. In Section 2 we introduce the time discrete Cahn–Hilliard system with double-obstacle free energy and its relaxation using Moreau–Yosida relaxation. We further summarize results from [14]. In Section 3 we apply proofs from [18] to obtain an $L^1(\Omega)$ bound and based on this an $L^\infty(\Omega)$ bound on the constraint violation. A numerical validation is carried out in Section 4, where in fact we observe higher rates than proven before. For this better rate we give an argumentation in Section 5.

2. The Cahn–Hilliard system with double-obstacle free energy

In the following, let $\Omega \subset \mathbb{R}^n$, $n \in \{2,3\}$ denote an open bounded domain, that fulfils the cone condition, see [2]. Its outer normal we denote by ν_Ω.

We further use usual notation for Sobolev spaces defined on Ω, see [2], i.e. $W^{k,p}(\Omega)$ denotes the space of functions that admit weak derivatives up to order k that are Lebesgue-integrable to the power p. For $p = 2$ we write $H^k(\Omega) := W^{k,2}(\Omega)$ and for $k = 0$ we write $L^p(\Omega) := W^{0,p}(\Omega)$. For $v \in W^{k,p}(\Omega)$ its norm is denoted by $\|v\|_{W^{k,p}(\Omega)}$.

Moreover we introduce

$$\mathcal{K} = \{v \in H^1(\Omega) \,|\, |v| \le 1 a.e.\},$$
$$V_0 = \{v \in H^1(\Omega) \,|\, (v,1) = 0\}.$$

For a fixed time t we consider an alloy consisting of two components A and B and we are interested in the evolution of this alloy over time. For the description of the distribution of the two components we introduce a phase field φ that serves as a binary indicator function in the sense, that $\varphi(x) = 1$ indicates pure fluid of component A at point $x \in \Omega$, while $\varphi(x) = -1$ indicates pure fluid of component B. We further assume, that the transition zone Γ_ϵ between A and B is of positive thickness, proportional to ϵ, and that both components are mixed therein. The phase field admits values from the interval $(-1,1)$ in this region.

We introduce the Ginzburg–Landau energy of the system by

$$GL(\varphi) = \int_\Omega \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{\epsilon}W(\varphi)\,dx.$$