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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

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

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

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

Here $W(\varphi)$ is the so called free energy density and is of double well type, i.e. it admits exactly two minima at ± 1 and is positive everywhere else. We denote the first variation of GL by

$$\mu := -\epsilon\Delta\varphi + \epsilon^{-1}W'(\varphi)$$

and introduce a mass conserving gradient flow with a mobility or diffusivity $b(\varphi)$ depending on the phase field as

$$\partial_t\varphi = \operatorname{div}(b(\varphi)\nabla\mu), \tag{1}$$

$$-\epsilon\Delta\varphi + \epsilon^{-1}W'(\varphi) = \mu. \tag{2}$$

We supplement (1)–(2) with appropriate initial data $\varphi_0 \in \mathcal{K}$ and boundary data $\nu_\Omega \cdot \nabla\varphi = \nu_\Omega \cdot \nabla\mu = 0$ on $\partial\Omega$. This system is introduced in [7] and is called Cahn–Hilliard system.

Specific choices of $b(\varphi)$ and $W(\varphi)$ give different analytical difficulties. Here we restrict to the case of non degenerate mobility $b(\varphi) \geq \theta$, for some $\theta > 0$, and for simplicity to constant mobility $b(\varphi) \equiv 1$.

For the free energy we choose the double-obstacle free energy introduced in [23] and analytically investigated in [5]. It has the form

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

Since this W is not smooth, (2) here has the form of a variational inequality, see Definition 1, where we state the precise formulation of the Cahn–Hilliard system with constant mobility and double-obstacle free energy.

Definition 1. *Let $\Omega \subset \mathbb{R}^n$, $n \in \{2,3\}$, denote a given bounded domain $I = (0,T]$, $T > 0$ denote a given time interval. $\varphi_0 \in \mathcal{K}$ is a given initial phase field.*

Then the Cahn–Hilliard system with constant mobility and double-obstacle free energy consists in finding a phase field φ and a chemical potential μ such that

$$\begin{aligned} \varphi \in H^1(0,T,(H^1(\Omega))^\star) \cap L^\infty(0,T,H^1(\Omega)), \\ \mu \in L^2(0,T,H^1(\Omega)), \\ \varphi(t) \in \mathcal{K} \quad \forall t \in (0,T), \\ (\varphi_t, v) + (\nabla\mu, \nabla v) = 0 \quad \forall v \in H^1(\Omega), \\ \epsilon(\nabla\varphi, \nabla v - \nabla\varphi) - \epsilon^{-1}(\varphi, v-\varphi) \geq (\mu, v-\varphi) \quad \forall v \in \mathcal{K}, \\ \nu_\Omega \cdot \nabla\varphi = 0 \quad \text{on } \partial\Omega, \\ \nu_\Omega \cdot \nabla\mu = 0 \quad \text{on } \partial\Omega, \\ \varphi(0) = \varphi_0. \end{aligned} \tag{3}$$

This system is first investigated in [5]. We state the existence and regularity results here.

Theorem 2 ([5]). *There exists a unique solution φ, μ to (3) fulfilling $\varphi \in L^2(0,T;H^2(\Omega))$, $\partial_{\nu_\Omega}\varphi = 0$ on $\partial\Omega$ for a.e. t. It further holds $\forall t > 0$ $\min(\sqrt{t},1)\|\varphi(t)\|_{H^2(\Omega)} \leq C(\varphi_0)$, and $\min(\sqrt{t},1)\|\mu(t)\|_{H^1(\Omega)} \leq C(\varphi_0)$.*

In this work we deal with the time discrete variant of (3). For this let $0 = t_0 < t_1 < \ldots < t_{k-1} < t_k < \ldots < t_M = T$ denote a decomposition of $I = (0,T]$ with time step size $\tau^k = t_k - t_{k-1}$.

Then the time discrete variant of (3) in weak form consist of finding $(\varphi^\star,\mu^\star)\in H^1(\Omega)\times H^1(\Omega)$ fulfilling

$$(\varphi^\star,v)+\tau^k(\nabla\mu^\star,\nabla v)=(\varphi^{k-1},v)\qquad \forall v\in H^1(\Omega), \tag{4}$$

$$\epsilon(\nabla\varphi^\star,\nabla v-\nabla\varphi^\star)-\epsilon^{-1}(\varphi^{k-1},v-\varphi^\star)\geq(\mu^\star,v-\varphi^\star)\qquad \forall v\in\mathcal{K}. \tag{5}$$

We further introduce a parameter $s\gg 0$ and the penalising function

$$\lambda(\varphi)=\lambda_+(\varphi)+\lambda_-(\varphi):=\max(0,\varphi-1)+\min(0,\varphi+1),$$

and define the outer approximation, [13], of (4)–(5) as follows:
Find $(\varphi^s,\mu^s)\in H^1(\Omega)\times H^1(\Omega)$ fulfilling

$$(\varphi^s,v)+\tau^k(\nabla\mu^s,\nabla v)=(\varphi^{k-1},v)\qquad \forall v\in H^1(\Omega), \tag{6}$$

$$\epsilon(\nabla\varphi^s,\nabla v)+\epsilon^{-1}(s\lambda(\varphi^s),v)-\epsilon^{-1}(\varphi^{k-1},v)=(\mu^s,v)\qquad \forall v\in H^1(\Omega). \tag{7}$$

Then the following result holds.

Theorem 3 ([14, Thm. 3.2, Thm. 4.1,Thm. 4.2, Lem. 4.3, Thm. 4.4])**.** *There exist unique solutions $\varphi^\star,\mu^\star$ to (4)–(5) and φ^s,μ^s to (6)–(7). Moreover*

$$(\varphi^s,\mu^s)\to(\varphi^\star,\mu^\star)\ \text{in}\ H^1(\Omega),$$

and there exists a constant $C>0$ independent of s such that

$$\|\varphi_s\|_{H^1(\Omega)}+s\|\lambda(\varphi_s)\|_{L^2(\Omega)}+\|\mu_s\|_{H^1(\Omega)}\leq C.$$

Remark 4. *We introduce a free energy density $W^s(\varphi)=\frac{1}{2}(1-\varphi^2)+\frac{s}{2}\lambda(\varphi)^2$. Then (7) can also be obtained as time discretization of (1)–(2) with this free energy. However, we note that W^s is not a valid free energy in the sense that its minima are located at $\theta=\pm\left(1+\frac{s}{s-1}\right)$ and attain negative values. After shifting W^s to have non negative values and scaling its argument by θ, this W^s might be regarded as a new type of free energy.*

From the point of treating variational inequalities, (7) is an outer approximation [13] of (5), while the logarithmic free energy proposed in [7] can be regarded as an inner approximation.

3. An L^∞ bound on the constraint violation

In this section we follow the approach in [18, Sec. 2]. Using the uniform boundedness of φ^s and μ^s from Theorem 3 we first derive $L^1(\Omega)$ bounds for the constraints violation $\lambda(\varphi^s)$ that we later use to derive a first bound on $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$.

Note that from regularity theory for the Laplace operator with Neumann boundary data, see e.g. [24], we have $\varphi^s\in H^2(\Omega)$ and from (7) and Theorem 3 it follows that $\|\varphi^s\|_{H^2(\Omega)}$ is uniformly bounded in s. From Sobolev embedding theory we further have $H^2(\Omega)\hookrightarrow C^{0,\beta}(\overline{\Omega})$ for $\beta<2-\frac{n}{2}$, and thus indeed $\lambda(\varphi^s)\in L^\infty(\Omega)$. From Theorem 3 we further have $\lambda(\varphi^s)\to 0$ for $s\to\infty$, compare also the discussion in [12, Rem. 6].

Theorem 5. *There exists $C>0$ independent of s, such that for $s\to\infty$ it holds*

$$\|\lambda(\varphi^s)\|_{L^1(\Omega)}\leq Cs^{-1}.$$

Proof. We test (6) with $v\equiv\mu^s$, (7) with $v\equiv\varphi^s$ and add the two equations yielding

$$\begin{aligned}\epsilon^{-1}s(\lambda(\varphi^s),\varphi^s)&=-\tau^k\|\nabla\mu^s\|^2+(\varphi^{k-1},\mu^s)-\epsilon\|\nabla\varphi^s\|^2+\epsilon^{-1}(\varphi^{k-1},\varphi^s)\\&\leq C\end{aligned}$$

with a $C>0$ independent of s by the uniform boundedness of φ^s and μ^s in $H^1(\Omega)$.

By noting $\varphi^s > 1 \Leftrightarrow \lambda_+(\varphi^s) > 0$ and $\varphi^s < -1 \Leftrightarrow \lambda_-(\varphi^s) < 0$, we further have

$$\int_\Omega \lambda_+(\varphi^s)\varphi^s\,dx \geq \int_\Omega |\lambda_+(\varphi^s)|\,dx, \quad \int_\Omega \lambda_-(\varphi^s)\varphi^s\,dx \geq \int_\Omega |\lambda_-(\varphi^s)|\,dx,$$

and thus

$$\epsilon^{-1}s\|\lambda(\varphi^s)\|_{L^1(\Omega)} \leq \epsilon^{-1}s(\lambda(\varphi^s),\varphi^s) \leq C$$

which completes the proof. □

We next derive a bound on $\|\lambda(\varphi^s)\|_{L^\infty}$ in terms of $\|\lambda(\varphi^s)\|_{L^1(\Omega)}$. Here we follow [15, Thm. 3.7], where [18, Thm. 2.4] is adapted.

Theorem 6. *It holds*

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \leq C(\Omega,n,\beta)\|\lambda(\varphi^s)\|_{L^1(\Omega)}^{\frac{\beta}{\beta+n}}$$

Proof. From $\varphi^s \in H^2(\Omega)$ we have the Hölder continuity of $\varphi^s \in C^{0,\beta}(\bar\Omega)$ for $\beta < 2 - \frac{n}{2}$, and thus there exists $C_\beta > 0$ independent of s with $\|\varphi^s\|_{C^{0,\beta}(\Omega)} \leq C_\beta$.

For fixed s we set $G^+ = \{x \in \Omega \,|\, \varphi^s(x) \geq 1\}$ and define $x_{\max} \in G^+$ to satisfy

$$\varphi^s(x_{\max}) - 1 = \|\varphi^s - 1\|_{L^\infty(G^+)}.$$

We set $G^- = \{x \in \Omega \,|\, \varphi^s(x) \leq -1\}$ and define $x_{\min} \in G^-$ to satisfy

$$-(\varphi^s(x_{\min}) + 1) = \|\varphi^s + 1\|_{L^\infty(G^-)}.$$

Now either $\varphi^s(x_{\max}) - 1 \equiv \|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$ or $-(\varphi^s(x_{\min})+1) \equiv \|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$ holds. W.l.o.g. we assume $\varphi^s(x_{\max}) - 1 \equiv \|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$ and in the following work in G^+.

From the definition of Hölder continuity we have

$$\varphi^s(x) - 1 \geq \varphi^s(x_{\max}) - 1 - \|\varphi^s\|_{C^{0,\beta}(\Omega)}|x_{\max} - x|^\beta.$$

Thus, for $|x_{\max} - x| \leq \left(\frac{\varphi^s(x_{\max})-1}{2C_\beta}\right)^{1/\beta}$

$$\varphi^s(x) - 1 \geq \frac{1}{2}(\varphi^s(x_{\max}) - 1) > 0$$

holds.

The domain Ω satisfies the cone condition. Thus there exists a cone $K_r(x_{\max}) := K(x_{\max}) \cap B(x_{\max}, r)$ of radius r and with vertex $x_{\max}$ such that $K_r(x_{\max}) \subset \Omega$. Hence the cone $K_R(x_{\max})$ with $R := \min\left(r, \left(\frac{\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}}{2C_\beta}\right)^{1/\beta}\right)$ is contained in G^+.

From this we conclude

$$\begin{aligned}
\|\lambda(\varphi^s)\|_{L^1(\Omega)} &\geq \int_{K_R(x_{\max})} \varphi^s - 1\,dx \\
&\geq \int_{K_R(x_{\max})} \frac{1}{2}(\varphi^s(x_{\max}) - 1)\,dx \\
&= \frac{|K_R(x_{\max})|}{2}\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \\
&\geq C(\Omega,n)\left(\frac{\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}}{2C_\beta}\right)^{n/\beta}\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \\
&= C(\Omega,n,\beta)\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}^{\frac{n+\beta}{\beta}}.
\end{aligned}$$

□

Corollary 7. *From Theorem 6 we have the following L^∞ bounds for the violation of the constraint $|\varphi| \le 1$.*

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \le \begin{cases} Cs^{-1/3+\gamma} & \text{if } n = 2, \\ Cs^{-1/7+\gamma} & \text{if } n = 3, \end{cases}$$

where $0 < \gamma \ll 1$.

Proof. It holds

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \le C\|\lambda(\varphi^s)\|_{L^1(\Omega)}^{\frac{\beta}{n+\beta}} \le Cs^{-\frac{\beta}{n+\beta}}.$$

For $n = 2$ we have $\beta < 1$ and thus the first claim.
For $n = 3$ we have $\beta < \frac{1}{2}$ and thus the second claim. □

Remark 8. *In* (7) *we use the violation $\lambda(\varphi^s)$ as penalisation for the outer approximation of the variational inequality* (5)*. The function λ is Lipschitz continuous, i.e. $\lambda \in C^{0,1}(\mathbb{R})$. We introduce smoother penalisations by using higher powers of λ, i.e. for $k \ge 2$ we define*

$$\lambda_k(\varphi^s) := \lambda(\varphi^s)|\lambda(\varphi^s)|^{k-2}.$$

Note that $\lambda_2(\varphi^s) \equiv \lambda(\varphi^s)$ and that it holds $\lambda_k \in C^{k-2,1}(\mathbb{R})$.

Let us argue this regularity. First it is clear that λ_k is infinitely often continuously differentiable away from ± 1. Let us concentrate on the case $+1$. The regularity at -1 only involves additional minus signs. Then for $x \in B_1(+1)$ we have $\lambda_k(x) = \max(0, x-1)^{k-1}$. This is continuously differentiable for $x > +1$ and for $x < +1$ and $\lim_{x \to +1} \lambda_k'(x) = 0$. The derivative can be written as $\lambda_k'(x) = (k-1)\max(0, x-1)^{k-2}$. This can be iterated until $\lambda^{(k-2)}(x) = (k-1)(k-2)\cdots 2\max(0, x-1)$ which then still is Lipschitz continuous.

Further we have at least $\varphi^s \in H^1(\Omega) \hookrightarrow L^q(\Omega)$ for $q \le 6$ if $n \equiv 3$ and $q < \infty$ for $n \equiv 2$. Thus for $k \le 7$ if $n \equiv 3$ and $k < \infty$ if $n \equiv 2$ we have $\lambda_k(\varphi^s) \in L^1(\Omega)$ and by iterating Sobolev embeddings and L^p-regularity theory for the Laplace operator ([20]) we obtain the required Hölder continuity of φ^s.

Using λ_k instead of λ in (7) *leads to the same results, but with λ substituted by λ_k. Especially we obtain*

$$\|\lambda_k(\varphi^s)\|_{L^\infty(\Omega)} = \|\lambda(\varphi^s)^{k-1}\|_{L^\infty(\Omega)} \le Cs^{-\frac{\beta}{n+\beta}} \tag{8}$$

and thus

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \le Cs^{-\frac{\beta}{(n+\beta)(k-1)}}$$

Such penalisations with smoother functions might be of interest for optimal control problems, [15, 16], where sufficient differentiability properties are required, or in the context of model order reduction using proper orthogonal decomposition, [25].

3.1. The fully discrete case. We assume, that Ω is polygonally bounded and thus can be represented exactly by a finite number of triangles if $n = 2$, resp. tetrahedrons if $n = 3$. We introduce a subdivision $\mathcal{T}$ of Ω using triangles, resp. tetrahedrons, and define the space of piecewise linear and globally continuous finite elements as

$$V_h = \{v \in C(\bar{\Omega}) \,|\, v|_T \in P^1(T)\, \forall T \in \mathcal{T}\} = \text{span}\{\phi_i \,|\, i = 1, \dots, N\},$$

where $P^1(T)$ denotes the space of all polynomials defined on T up to order 1. Note that functions from V_h are Hölder continuous with exponent $\beta < 1$.

The discrete counterparts φ_h^s, μ_h^s of φ^s, μ^s then fulfil the equations

$$(\varphi_h^s, v) + \tau^k(\nabla\mu_h^s, \nabla v) = (\varphi^{k-1}, v) \qquad \forall v \in V_h, \tag{9}$$

$$\epsilon(\nabla(\varphi_h^s, \nabla v) + \epsilon^{-1}\Lambda(\varphi_h^s, v) - \epsilon^{-1}(\varphi^{k-1}, v) = (\mu_h^s, v) \qquad \forall v \in V_h, \tag{10}$$

where we investigate three choices for the numerical treatment of the penalisation term $\Lambda_k(\varphi_h^s, v)$. Using linear elements the term $\Lambda(\varphi_h^s, v) = \Lambda_E(\varphi_h^s, v) := (s\lambda(\varphi_h^s), v)$ can be evaluated exactly. Another possibility is to use the Lagrangian interpolation I for $\lambda(\varphi_h^s)$, i.e. $\Lambda(\varphi_h^s, v) = \Lambda_I(\varphi_h^s, v) := (sI(\lambda(\varphi_h^s)), v)$. As last variant we investigate an evaluation using lumping, i.e. $\Lambda(\varphi_h^s, v) = \Lambda_L(\varphi_h^s, v) := (s\lambda(\varphi_h^s), v)^h$, where $(v, w)^h$ is defined as

$$(v, w)^h := \sum_{i=1}^{N} (1, \phi_i) v(x_i) w(x_i),$$

and x_i stands for the vertices of $\mathcal{T}$.

Note that $|I(\lambda(\varphi_h^s))| \geq |\lambda(\varphi_h^s)|$ and $\|I(\lambda(\varphi_h^s))\|_{L^\infty(\Omega)} \equiv \|\lambda(\varphi_h^s)\|_{L^\infty(\Omega)}$ due to the linear finite elements that we use.

Using the different variants of Λ the results from Section 3 stay valid for the fully discrete case, with small changes that we comment on next.

For Λ_E no changes are required. For Λ_I and Λ_L we obtain from Theorem 5

$$\epsilon^{-1}s\|\lambda(\varphi_h^s)\|_{L^1(\Omega)} \leq \epsilon^{-1}s\|I(\lambda(\varphi_h^s))\|_{L^1(\Omega)} \leq C.$$

The according $L^\infty(\Omega)$ bounds for $\lambda(\varphi_h^s)$ in Theorem 6 then follow immediately.

4. Numerical validation

In this section we perform numerical tests to validate the bounds that we found in Theorem 6.

We perform simulations in two and three space dimensions, using $\Omega = (0, 1)^n$, i.e. the unit square for $n = 2$, and the unit cube for $n = 3$.

We perform one time step of (6)–(7) and measure the violation $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$. The parameter are given as $\epsilon = 0.01$ and $\tau = 0.01$ if $n = 2$ and $\epsilon = 0.04$ and $\tau = 0.01$ if $n = 3$. The initial phase field φ_0 is defined as

$$\varphi_0(x) = \begin{cases} 1 & \text{if } z \geq \frac{\pi}{2}, \\ -1 & \text{if } z \leq -\frac{\pi}{2}, \\ \sin(z) & \text{else,} \end{cases}$$

where $z = \epsilon^{-1}(\|x - m\| - r)$, and $m = (0.5, 0.5)$ for $n = 2$ and $m = (0.5, 0.5, 0.5)$ if $n = 3$. This defines a sphere with radius $r = 0.25$. Note that the sine is the principle shape of the phase field across the interface for the double-obstacle free energy [11].

We adapt the mesh for the phase field and the chemical potential by using the reliable and efficient residual based error estimator proposed in [14]. Here we only use the norm of the jumps of the normal derivatives of φ_h^s and μ_h^s across edges for $n = 2$, resp. faces for $n = 3$, which contains the main part of the indicator [8]. For the marking of cells we follow [14], i.e. we use the procedure proposed by Dörfer [10].

We perform the usual "solve→estimate→mark→refine" cycle three times for each value of s and reuse the final mesh as initial mesh for the next larger value of s. In Figure 1 we show a typically mesh obtained by this adaptive solving procedure.

The non linear system (9)–(10) is solved using Newton's method and the linear systems are solved directly. We solve the system up to a residuum of 10^{-6} and

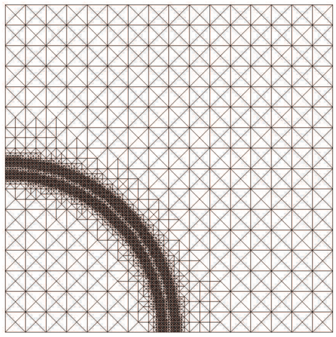

FIGURE 1. One quarter of the computational domain for the 2d simulation.

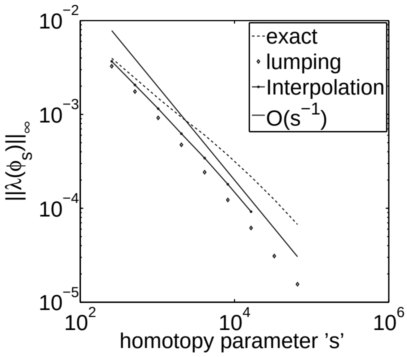

FIGURE 2. The violation of the bound $|\varphi| \leq 1$ for penalisation with λ_2, and the different numerical treatments, i.e. exact evaluation, lumping and interpolation. Note that Newton's method failed in calculating the solution for larger values of s if interpolation is used.

allow at most 100 Newton steps. The implementation is done in C++ using the finite element toolbox FEniCS [21] with the PETSc [4] linear algebra back end and the MUMPS [3] direct solver.

Experiments in two space dimensions. In two space dimensions we investigate the three cases of numerical treatment of the penalisation $\lambda(\varphi^s)$ as proposed in Section 3.1, namely the exact integration, the interpolation case and the lumping case.

In Figure 2 we present numerical results. We show the violation $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$ for the different numerical treatments of terms involving λ.

In the case of exact evaluation and lumping evaluation, Newton's method is able to find a solution with the desired tolerance 10^{-6} in much less than the allowed 100 Newton steps, typically 5-10 steps, for all tested values of s, and we observe that the theoretical bound from Theorem 6, i.e. $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \leq Cs^{-1/3}$, holds. However, we observe a significant higher rate, i.e. $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \leq Cs^{-1}$, than expected from the results of Theorem 6. This can not be explained by the theory so far. In Section 5 we give a hint how these rates might be argued.

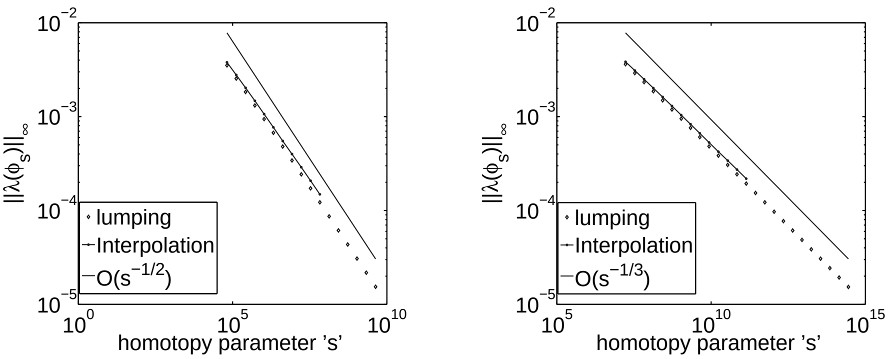

FIGURE 3. The violation of the bound $|\varphi| \leq 1$ for penalisation with λ_k, $k = 3, 4$ (left to right) and the different numerical treatments, i.e. lumping and interpolation. Note that in both cases, Newton's method fails in calculating the solution for larger values of s if interpolation is used.

Comparing the three ways of evaluating the penalisation, in the case of exact integration we have a slightly higher violation of the constraints, and the rate is only attained for large values of s.

When interpolation is used for the evaluation, we observe that, for larger values of s, Newton's method is not able to find a solution with the desired tolerance within the maximum allowed number of iterations. While e.g. for $s = 16384$ after the first step the residuum is reduced from 1.4 to 6e-4, the subsequent Newton steps only converge linearly with a linear rate of 0.95, resulting in a residuum of 5e-6 after 100 steps. In general Newton's method requires more steps when interpolation is applied than when the other variants are used. The reason for this behaviour stays unclear. Especially we note, that the condition number of the linear systems is nearly independent of the way of evaluating the non-linearity and that all integrals are evaluated exactly.

As next test we investigate $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)}$ when λ_k for $k > 2$ is used for penalisation as proposed in Remark 8. Here we do not perform exact integration.

Also in the case of higher powers of λ the theoretical bounds are attained. Again we observe that Newton's method fails in finding the solution for large values of s if interpolation is used, while with lumped evaluation the solution is always found. Note that to obtain comparable violations for λ_k we need larger values of s.

Experiments in three space dimensions. In three dimensions we only investigate lumping and interpolation as treatment of the term with λ and again we use λ_k for $k = 2, 3, 4$.

In Figure 4 we show the numerical results. Again we obtain the expected bounds from Theorem 6 and as in the 2D case even a higher rate. Also using interpolation Newton's method fails in finding the unique solution for larger values of s.

5. An argumentation for the higher rate

In Section 4 we have seen that the theoretical bounds, as shown in Theorem 6, are valid in a numerical example. In this example we found, that even a higher rate, i.e. $\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \leq Cs^{-1}$, is obtained for $n = 2, 3$. This is not covered by the developed theory. In [18, Ass. 2.13] a structural assumption on the active set

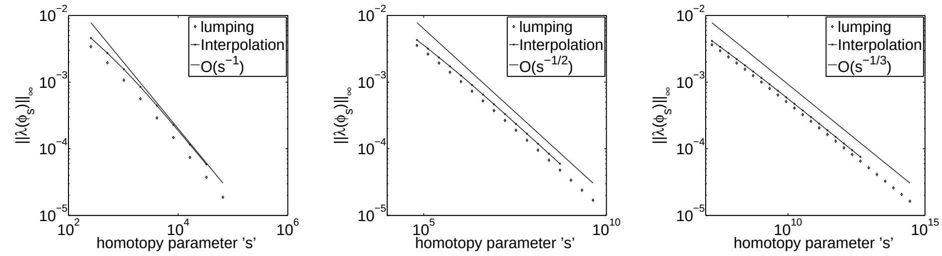

FIGURE 4. Numerical results for three space dimensions and with λ_k, $k = 2, 3, 4$ (left to right). The proposed convergence rate is obtained and again in the case of interpolation of λ Newton's method fails in finding the solution for large values of s.

of the regularized problem is used to argue higher rates and we next follow their argumentation.

It is reasonable to assume that the integral over Ω with respect to the measure $\lambda^\star$, which is the Lagrange multiplier associated with the inequality constraint $|\varphi^\star| \leq 1$ in (4)–(5), is of the same order as the volume of Ω. This is a reasonable assumption as $\lambda^\star$ is concentrated on the active set for the inequality constraint $|\varphi| \leq 1$, which in our setting describes the pure phases. This assumption means that for $x \in \Omega$ and the ball $B_R(x)$ with radius $R > 0$ there exists a constant $0 < K < \infty$ independent of R and x such that

$$\int_{B_R(x)} d\lambda^\star \leq K R^n \tag{11}$$

holds.

We further have the weak convergence $\lambda(\varphi^s) \rightharpoonup \lambda^\star$, [17], and thus especially

$$\int_\Omega d|\lambda(\varphi^s)| := \int_\Omega |\lambda(\varphi^s)| \, dx \to \int_\Omega d\lambda^\star.$$

It is thus reasonable to assume, that a similar behaviour as (11) holds for $\lambda(\varphi^s)$ and we state the following assumption.

For $x \in \Omega$ we assume that there exists $0 < K < \infty$, independent of x, R, and s such that

$$\int_{B_R(x)} d\lambda(\varphi^s) \leq K R^n \tag{12}$$

holds.

However, from this assumption we can now directly obtain the desired rate by dividing by R^n and taking the limit $R \to 0$ and obtain the observed rate

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \leq K s^{-1}.$$

Note that this bound is significantly better than the one shown in Theorem 6 and especially is independent of the dimension n of the domain Ω, as observed in Section 4, and of the Hölder exponent β of φ^s. We further stress, that a rigorous proof is left as an open question.

In the case of smoother penalisations we obtain

$$\|\lambda_k(\varphi^s)\|_{L^\infty(\Omega)} = \|\lambda^{k-1}(\varphi^s)\|_{L^\infty(\Omega)} \leq K s^{-1}$$

and thus

$$\|\lambda(\varphi^s)\|_{L^\infty(\Omega)} \le K s^{-\frac{1}{k-1}}$$

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