Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 288 (2015) 75–82
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Robustness of error estimates for phase field models at a class of topological changes

Sören Bartels*

Department of Applied Mathematics, University of Freiburg, Hermann-Herder-Str. 10, 79104 Freiburg, Germany

Available online 11 November 2014

Highlights

- Characterization of stability for phase field evolutions at singularities.
- Accuracy of numerical methods when particles vanish.
- Description of phase boundaries when topological changes occur.

Abstract

A priori and a posteriori error estimates for the numerical approximation of phase field models with a polynomial dependence on the inverse of the interface width as long as no topological changes occur have recently been derived. Numerical experiments show that they remain robust when topological changes of the interface take place. Based on an asymptotic expansion a lower bound for the principal eigenvalue of the linearized Allen–Cahn operator near a generic singularity is derived which explains this experimental observation.

Keywords: Allen–Cahn equation; Numerical approximation spectral estimate; Singularities; Scaling; Stability

1. Introduction

Phase field equations provide a flexible mathematical tool to describe the evolution of interfaces or surfaces in various processes such as crystal growth, multiphase flows, or crack propagation. In contrast to sharp interface models their numerical implementation can be realized with standard methods and they are capable of describing topological changes effectively. The simplest example is the Allen–Cahn equation

$$\partial_t u - \Delta u = -\varepsilon^{-2} f(u)$$

in which $\varepsilon > 0$ is a small parameter that describes the thickness of the diffuse interface that separates regions in which $u \approx \pm 1$ and f is the derivative of a double well potential, e.g., $f(u) = 2(u^3 - u)$. Fig. 1 displays snapshots of a simple but generic evolution leading to a generic topological change, i.e., a circular interface shrinks and disappears

* Tel.: +49 761203 5628; fax: +49 761203 5632.
E-mail address: bartels@mathematik.uni-freiburg.de.

http://dx.doi.org/10.1016/j.cma.2014.11.005
0045-7825/

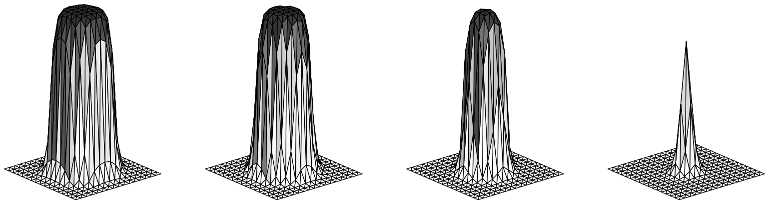

Fig. 1. Numerical experiment leading to a topological change. The circular interface that separates regions in which $u \approx \pm 1$ shrinks and collapses in finite time.

in finite time. Although the mathematical modeling of such events is unclear the agreement with experiments is quite remarkable. The topological change corresponds to a singularity in the evolution and the approximation properties of numerical methods may be critically affected. It is the aim of this article to provide a theoretical justification for the reliability of standard numerical methods at topological changes in a simple model situation.

Spectral estimates have recently been employed to derive error estimates of the form

$$\sup_{t\in[T_0,T_1]} \|u-u_h\| \le c_1\varepsilon^{-\sigma}(h^\alpha+\tau^\beta)\exp\left(c_2\int_{T_0}^{T_1} -\lambda_{AC}^-(t)\,dt\right) \tag{1.1}$$

for the numerical approximation of phase field models such as the Allen–Cahn equation cf. [1–4]. The negative part $\lambda_{AC}^- = \min\{\lambda_{AC},0\}$ of the principal eigenvalue λ_{AC} of the linearized Allen–Cahn operator

$$-\Delta + \varepsilon^{-2} f'(u(t))\,\mathrm{id}$$

about the exact solution at time t enters such estimates exponentially and thus logarithmic bounds for this quantity lead to useful estimates, cf. [4]. For the smooth evolution of developed interfaces it is known that the eigenvalue remains uniformly bounded from below [5–7] while for topological changes its modulus attains the square of the inverse of the interface thickness. Numerical experiments in [4] indicate that the modulus of the principal eigenvalue grows like $1/|t|,\ t<0$, prior to a topological change at $t=0$, before it attains the maximal absolute value proportional to ε^{-2}. Hence, an integration of it in time leads to a logarithmic bound which implies the robustness of the error estimate. It is the aim of this paper to provide theoretical support for such a scaling behavior.

For the mean curvature flow

$$V = -H$$

with a circle of radius $\sqrt{2}$ at $t=-1$ as initial data, the evolution is defined through $\dot{R} = -1/R$, i.e., $R(t) = \sqrt{2}|t|^{1/2}$ for $-1 \le t < 0$. The linearization of H in the class of circles is given by

$$H'(t) = -\frac{1}{R(t)^2} = -\frac{1}{2}|t|^{-1}$$

which shows that the linearization of the sharp interface model obeys the scaling property observed for the related phase field model. Since the Allen–Cahn problem approximates the mean curvature flow as the interface thickness tends to zero [8,9] we expect that a similar bound holds for the principal eigenvalue of the linearized Allen–Cahn operator. We adopt the techniques of [6] to give a proof of this statement under the following assumption.

Assumption A. The solution ϕ_ε of the Allen–Cahn problem in $B_2\times(-T,0)$ with $B_2 := B_2(0)\subset\mathbb{R}^2$, i.e., the function ϕ_ε that satisfies

$$\partial_t\phi_\varepsilon - \Delta\phi_\varepsilon = -\varepsilon^{-2} f(\phi_\varepsilon),$$

with $f(u) := 2(u^2-1)u$ and $0<\varepsilon<1$, is for $t \le -\varepsilon^2\log(\varepsilon^{-1})$ given by

$$\phi_\varepsilon(r,t) = \tanh\big((r-\sqrt{2}|t|^{1/2})/\varepsilon\big) + \varepsilon^2 q_\varepsilon(r,t) \tag{1.2}$$

with a function q_ε that satisfies

$$|q_\varepsilon(r,t)| \le c_0|t|^{-1}. \tag{1.3}$$

The assumption is motivated by the expansion

$$\phi_\varepsilon(x,t) = \tanh(d/\varepsilon) + \varepsilon^2 H^2 \xi(d/\varepsilon) + \mathcal{O}(\varepsilon^3)$$

in which d denotes the signed distance to the interface, H is the mean curvature of the interface, and ξ is a smooth function, cf. [10,9] for details. This assumption is confirmed by numerical experiments reported in Appendix A and is expected to be justifiable rigorously by an appropriate construction of super- and subsolutions. The assumption enables us to prove the asserted result.

Theorem 1.1. *Suppose that Assumption A holds. Then the estimate*

$$\lambda_{AC}(t) := \inf_{0\neq\psi\in H^1(B_2)} \frac{\int_{B_2} |\nabla\psi|^2 + \varepsilon^{-2} f'\big(\phi_\varepsilon(r,t)\big)\psi^2 dx}{\|\psi\|^2_{L^2(B_2)}} \geq -C_{AC}|t|^{-1}$$

holds for $t \in [-T, -\varepsilon^2\log(\varepsilon^{-1})]$ with an ε-independent constant $C_{AC} \geq 0$.

With this bound for λ_{AC} and the unconditional estimate $\lambda_{AC}(t) \geq -C'_{AC}\varepsilon^{-2}$, which follows from considering $\psi = 1$ in the definition of λ_{AC}, the argument of the exponential factor in (1.1) with $T_0 = -1$ and $T_1 = 0$ satisfies

$$\begin{aligned}\int_{T_0}^{T_1} -\lambda_{AC}^-(t)dt &\leq C_{AC}\int_{-1}^{-\varepsilon^2\log(\varepsilon^{-1})} |t|^{-1}dt + C'_{AC}\int_{-\varepsilon^2\log(\varepsilon^{-1})}^{0} \varepsilon^{-2}dt \\ &= -C_{AC}\log(|t|)\big|_{-1}^{-\varepsilon^2} + C'_{AC}\log(\varepsilon^{-1}) \leq C''_{AC}\log(\varepsilon^{-1}).\end{aligned}$$

This implies that the error bound depends polynomially on ε^{-1} in the considered situation.

Remarks 1.1. (i) Terms of order ε can be included in (1.2) as long as one restricts to $t \leq -\varepsilon^2\log(\varepsilon^{-1})^2$. This however is not sufficient to prove robust stability estimates.

(ii) The lower bound of Theorem 1.1 is expected to hold also in three space dimensions.

(iii) Since interfaces always become circular in two-dimensional Allen–Cahn evolutions, cf. [11], the considered situation of Assumption A is generic.

(iv) An equivalent statement to that of Theorem 1.1 is to say that $\lambda_{AC}(t) \geq -cH_m^2(t)$, where $H_m(t)$ is the maximal curvature of the interface.

2. Allen–Cahn profile on a bounded interval

Given $t \leq -\varepsilon^2\log(\varepsilon^{-1})$ we consider the operator

$$\mathcal{L}^0_{\varepsilon,t} := -d^2/dz^2 + f'(\theta_0) \quad \text{in } I_{\varepsilon,t} := (-|t|^{1/2}/(\sqrt{2}\varepsilon), 1/\varepsilon)$$

subject to homogeneous Neumann boundary conditions on $\partial I_{\varepsilon,t}$ and define

$$L^0_{\varepsilon,t}(\Phi,\Psi) := \int_{I_{\varepsilon,t}} \Phi'\Psi' + f'(\theta_0)\Phi\Psi dz$$

for $\Phi, \Psi \in H^1(I_{\varepsilon,t})$. The function $\theta_0(z) := \tanh(z) = (e^z - e^{-z})/(e^z + e^{-z})$ solves

$$-\theta'' + f(\theta) = 0, \qquad \theta(0) = 0, \qquad \lim_{z\to\pm\infty}\theta(z) = \pm 1.$$

Moreover, $\theta_0'(z) = 1/\cosh^2(z)$ and $\theta_0''(z) = -2\sinh(z)/\cosh^3(z)$ satisfy

$$0 < \theta_0'(z) \leq 4e^{-2|z|} \quad \text{and} \quad |\theta_0''(z)| \leq 8e^{-2|z|}. \tag{2.1}$$

Lemma 2.1. *The principal eigenvalue λ_1^0 of $\mathcal{L}^0_{\varepsilon,t}$ satisfies*

$$-c_4 e^{-(1+2\sqrt{2})|t|^{1/2}/\varepsilon} \leq \lambda_1^0 = \inf_{0\neq\Psi\in H^1(I_{\varepsilon,t})} \frac{L^0_{\varepsilon,t}(\Psi,\Psi)}{\|\Psi\|^2_{L^2(I_{\varepsilon,t})}} \leq c_1 e^{-2\sqrt{2}|t|^{1/2}/\varepsilon},$$

where $c_1, c_4 > 0$ are ε-independent constants.

Proof. The shifted operator $\mathcal{L}^0_{\varepsilon,t} + \max_{I_{\varepsilon,t}} |f'(\theta_0)|$ is self-adjoint and positive definite so that $-\max_{I_{\varepsilon,t}} |f'(\theta_0)| \le \lambda_1^0$. Integration by parts, $\mathcal{L}^0_{\varepsilon,t}\theta_0' = (-\theta_0'' + f(\theta_0))' = 0$, and (2.1) show

$$\lambda_1^0 \le \beta^2 L^0_{\varepsilon,t}(\theta_0', \theta_0') = \beta^2 \theta_0'\theta_0''\big|_{-|t|^{1/2}/(\sqrt{2}\varepsilon)}^{1/\varepsilon} \le \beta^2 64 e^{-4|t|^{1/2}/(\sqrt{2}\varepsilon)} =: c_1 e^{-2\sqrt{2}|t|^{1/2}/\varepsilon}, \tag{2.2}$$

where we used that $|t|^{1/2}/(\sqrt{2}\varepsilon) \le 1/\varepsilon$ and defined $\beta^2 := \|\theta_0'\|^{-2}_{L^2(I_{\varepsilon,t})} \le 1$. Set $m := \max\{f'(-1), f'(1)\} = 4$ and let $a_0 > 0$ be such that $f'(\theta_0(z)) \ge 3m/4$ for all $|z| \ge a_0$. Since a_0 is independent of ε we may assume that $\pm(a_0+1) \in I_{\varepsilon,t}$. Owing to (2.2) we may assume that $\lambda_1^0 \le m/4$. Then, the positive eigenfunction Ψ_1^0 satisfies

$$-(\Psi_1^0)'' + (f'(\theta_0) - \lambda_1^0)\Psi_1^0 = 0,$$

with $f'(\theta_0) - \lambda_1^0 \ge m/2$ in $I_{\varepsilon,t} \setminus [-a_0, a_0]$. Since $\|\Psi_1^0\|_{L^2(I_{\varepsilon,t})} = 1$ we may choose $a_0' \in [a_0, a_0+1]$ such that $\Psi_1^0(\pm a_0') \le 1$. A comparison argument with the functions

$$\Phi_+(z) :=: \Psi(a_0') \frac{\cosh\big(c(1/\varepsilon - z)\big)}{\cosh\big(c(1/\varepsilon - a_0')\big)}, \qquad \Phi_-(z) := \Psi(-a_0') \frac{\cosh\big(c(|t|^{1/2}/(\sqrt{2}\varepsilon) + z)\big)}{\cosh\big(c(|t|^{1/2}/(\sqrt{2}\varepsilon) - a_0')\big)},$$

where $c = \sqrt{m/2}$, shows that $\Psi_1^0(z) \le \Phi_+(z)$ for $z \ge a_0'$ and $\Psi_1^0(z) \le \Phi_-(z)$ for $z \le -a_0'$, cf. Lemma B.1 for details. We thus deduce that for $z \in I_{\varepsilon,t} \setminus [-(a_0+1), a_0+1]$ we have

$$\Psi_1^0(z) \le \Phi_\pm(z) \le 2e^{-c|z|}e^{ca_0'} \le 2e^{-c|z|}e^{c(a_0+1)} =: c_2 e^{-\sqrt{2}|z|}.$$

This, integration by parts, $\mathcal{L}^0_{\varepsilon,t}\theta_0' = 0$, and (2.1) imply

$$\lambda_1^0 \int_{I_{\varepsilon,t}} \Psi_1^0 \theta_0' dz = \int_{I_{\varepsilon,t}} (\mathcal{L}^0_{\varepsilon,t}\Psi_1^0)\theta_0' dz = \theta_0'' \Psi_1^0\big|_{-|t|^{1/2}/(\sqrt{2}\varepsilon)}^{1/\varepsilon} \ge -16 c_2 e^{-(\sqrt{2}+4)|t|^{1/2}/(\sqrt{2}\varepsilon)}.$$

It remains to prove a lower bound for $\int_{I_{\varepsilon,t}} \Psi_1^0\theta_0' dz$. Owing to $\theta_0' > 0$ it suffices to show that Ψ_1^0 is uniformly bounded from below in $(-a^*, a^*)$ for some a^* independent of ε. Since $\|\Psi_1^0\|_{L^2(I_{\varepsilon,t})} = 1$ and $\Psi_1^0(z) \le c_2 e^{-\sqrt{2}|z|}$, $|z| \ge a_0 + 1$, there exists an ε-independent number $a^* > 0$ such that

$$\int_{-a^*}^{a^*} |\Psi_1^0(z)|^2 dz \ge 1/2.$$

The coefficients of $\mathcal{L}^0_{\varepsilon,t} - \lambda_1^0$ are uniformly bounded so that an application of Harnack's inequality, cf., e.g., [12], to the identity

$$(\mathcal{L}^0_{\varepsilon,t} - \lambda_1^0)\Psi_1^0 = 0 \quad \text{in } (-a^*-1, a^*+1)$$

implies the existence of a constant $c_3 > 0$ such that

$$\inf_{z \in (-a^*, a^*)} \Psi_1^0(z) \ge c_3 \sup_{z \in (-a^*, a^*)} \Psi_1^0(z) \ge c_3 \left(\frac{1}{2a^*} \int_{-a^*}^{a^*} (\Psi_1^0)^2 dz \right)^{1/2} \ge c_3 \frac{1}{(4a^*)^{1/2}}.$$

This proves $\lambda_1^0 \ge -c_4 e^{-(1+2\sqrt{2})|t|^{1/2}/\varepsilon}$ and finishes the proof. □

3. Reduction to the one-dimensional situation

Under the assumptions on ϕ_ε stated in Assumption A, the estimation of λ_{AC} reduces to a one-dimensional problem. For $\psi \in C^1(B_2)$ we have

$$\int_{B_2} \varepsilon|\nabla\psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon)\psi^2 dx \ge 2\pi \int_{|t|^{1/2}/\sqrt{2}}^{1+\sqrt{2}|t|^{1/2}} \big(\varepsilon|\psi_r|^2 + \varepsilon^{-1} f'(\phi_\varepsilon)\psi^2\big) r dr.$$

The transformation $z = (r - \sqrt{2}|t|^{1/2})/\varepsilon$ and the rescaling $\Psi(z) := \varepsilon^{1/2}\psi(r)$ lead to

$$\int_{B_2} \varepsilon|\nabla\psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon)\psi^2 dx \geq \frac{2\pi}{\varepsilon}\int_{I_{\varepsilon,t}} \big(|\Psi_z|^2 + f'(\tilde{\phi}_\varepsilon)\Psi^2\big)\tilde{J}(z)dz =: \frac{2\pi}{\varepsilon} L_{\varepsilon,t}(\Psi,\Psi), \tag{3.1}$$

where $I_{\varepsilon,t} = \big(-|t|^{1/2}/(\sqrt{2}\varepsilon), 1/\varepsilon\big)$, $\tilde{J}(z) = \varepsilon z + \sqrt{2}|t|^{1/2}$, and $\tilde{\phi}_\varepsilon(z,t) = \phi_\varepsilon(\varepsilon z + \sqrt{2}|t|^{1/2}) = \theta_0(z) + \varepsilon^2\tilde{q}_\varepsilon(z,t)$ with $\tilde{q}_\varepsilon(z,t) = q_\varepsilon(\varepsilon z + \sqrt{2}|t|^{1/2}, t)$. Since

$$\|\psi\|^2_{L^2(B_2)} \geq 2\pi \int_{|t|^{1/2}/\sqrt{2}}^{1+\sqrt{2}|t|^{1/2}} \psi^2 r dr = 2\pi \int_{I_{\varepsilon,t}} \Psi^2\tilde{J}(z)dz.$$

Theorem 1.1 follows from the next lemma.

Lemma 3.1. *For $t \in [-T, -\varepsilon^2\log(\varepsilon^{-1})]$ the principal eigenvalue λ_1 of $L_{\varepsilon,t}$ defined in (3.1) satisfies*

$$-c_8\varepsilon^2|t|^{-1} \leq \lambda_1 = \inf_{0\neq\Psi\in H^1(I_{\varepsilon,t})} \frac{L_{\varepsilon,t}(\Psi,\Psi)}{\|\Psi\tilde{J}^{1/2}\|^2_{L^2(I_{\varepsilon,t})}} \leq c_6\varepsilon|t|^{-1},$$

where $c_6, c_8 > 0$ are ε-independent constants.

Proof. Let $\Psi \in H^1(I_{\varepsilon,t})$ and define $\widehat{\Psi} := \tilde{J}^{1/2}\Psi$. Noting $\Psi_z\tilde{J}^{1/2} = \widehat{\Psi}_z - \varepsilon\tilde{J}^{-1}\widehat{\Psi}/2$, where $\tilde{J}^{-1} := 1/\tilde{J}$, we deduce

$$\begin{aligned} L_{\varepsilon,t}(\Psi,\Psi) &= \int_{I_{\varepsilon,t}} \widehat{\Psi}_z^2 + f'(\tilde{\phi}_\varepsilon(z,t))\widehat{\Psi}^2 dz + \frac{\varepsilon^2}{4}\int_{I_{\varepsilon,t}} \tilde{J}^{-2}\widehat{\Psi}^2 dz - \varepsilon\int_{I_{\varepsilon,t}} \tilde{J}^{-1}\widehat{\Psi}\widehat{\Psi}_z dz \\ &= L^0_{\varepsilon,t}(\widehat{\Psi},\widehat{\Psi}) + \int_{I_{\varepsilon,t}} \big(f'(\tilde{\phi}_\varepsilon(z,t)) - f'(\theta_0(z))\big)\widehat{\Psi}^2 dz \\ &\quad + \frac{\varepsilon^2}{4}\int_{I_{\varepsilon,t}} \tilde{J}^{-2}\widehat{\Psi}^2 dz - \frac{\varepsilon}{2}\int_{I_{\varepsilon,t}} \tilde{J}^{-1}(\widehat{\Psi}^2)_z dz. \end{aligned}$$

A Taylor expansion of the quadratic function f' about θ_0 shows

$$f'\big(\tilde{\phi}_\varepsilon(z,t)\big) - f'\big(\theta_0(z)\big) = \varepsilon^2 f''(\theta_0)\tilde{q}_\varepsilon + f'''(\theta_0)(\varepsilon^2\tilde{q}_\varepsilon)^2/2 =: \varepsilon^2 r_\varepsilon \tag{3.2}$$

with $|r_\varepsilon| \leq c_5|t|^{-1}$ owing to (1.3). An integration by parts and $(\tilde{J}^{-1})_z = -\tilde{J}^{-2}\varepsilon$ lead to

$$-\int_{I_{\varepsilon,t}} \tilde{J}^{-1}(\widehat{\Psi}^2)_z dz = -\varepsilon\int_{I_{\varepsilon,t}} \tilde{J}^{-2}\widehat{\Psi}^2 dz - \tilde{J}^{-1}\widehat{\Psi}^2\big|^{1/\varepsilon}_{-|t|^{1/2}/(\sqrt{2}\varepsilon)}.$$

This implies

$$L_{\varepsilon,t}(\Psi,\Psi) = L^0_{\varepsilon,t}(\widehat{\Psi},\widehat{\Psi}) + \varepsilon^2\int_{I_{\varepsilon,t}} r_\varepsilon\widehat{\Psi}^2 dz - \frac{\varepsilon^2}{4}\int_{I_{\varepsilon,t}} \tilde{J}^{-2}\widehat{\Psi}^2 dz - \frac{\varepsilon}{2}\tilde{J}^{-1}\widehat{\Psi}^2\big|^{1/\varepsilon}_{-|t|^{1/2}/(\sqrt{2}\varepsilon)}. \tag{3.3}$$

We conclude with (2.1) and (2.2) that

$$\begin{aligned} \lambda_1 &= \inf_{\|\Psi\tilde{J}^{1/2}\|_{L^2(I_{\varepsilon,t})}=1} L_{\varepsilon,t}(\Psi,\Psi) \leq L_{\varepsilon,t}(\beta\tilde{J}^{-1/2}\theta_0', \beta\tilde{J}^{-1/2}\theta_0') \\ &\leq \beta^2 L^0_{\varepsilon,t}(\theta_0',\theta_0') + c_5\varepsilon^2|t|^{-1} + \beta^2\frac{\varepsilon}{2}\big(\theta_0'(-\sqrt{2}|t|^{1/2}/(2\varepsilon))\big)^2 \leq c_6\varepsilon|t|^{-1}, \end{aligned}$$

where we used that $e^{-2\sqrt{2}|t|^{1/2}/\varepsilon} \leq 1$ for ε sufficiently small. Let Ψ_1 be the positive eigenfunction corresponding to λ_1 with $\|\Psi_1\tilde{J}^{1/2}\|_{L^2(I_{\varepsilon,t})} = 1$ and note that Ψ_1 satisfies

$$-\tilde{J}^{-1}\frac{d}{dz}\big(\tilde{J}\frac{d}{dz}\Psi_1\big) + f'(\tilde{\phi}_\varepsilon(z,t))\Psi_1 = \lambda_1\Psi_1$$

in $I_{\varepsilon,t}$. We may assume that $\lambda_1 \le m/4$, and $f'(\tilde{\phi}_\varepsilon(z,t)) \ge 3m/4$ for $z \ge a_0$ with an ε-independent number $a_0 > 0$ such that $a_0 + 1 \le 1/\varepsilon$. Let $a_0' \in [a_0, a_0+1]$ such that $\Psi_1(a_0')\tilde{J}^{1/2}(a_0') \le 1$. Employing the comparison function

$$\Phi(z) = \Psi_1(a_0') \frac{\cosh\big(c(1/\varepsilon - z)\big)}{\cosh\big(c(1/\varepsilon - a_0')\big)},$$

where $c = \sqrt{m/2}$, we deduce that, cf. Lemma B.2 for details,

$$\Psi_1(z) \le c_7 e^{-\sqrt{2}z} \tilde{J}^{-1/2}(a_0').$$

With $\widehat{\Psi}_1 := \tilde{J}^{1/2}\Psi_1$ we deduce from (3.3) and Lemma 2.1 that

$$\begin{aligned} \lambda_1 = L_{\varepsilon,t}(\Psi_1, \Psi_1) &\ge L^0_{\varepsilon,t}(\widehat{\Psi}_1, \widehat{\Psi}_1) - c_5\varepsilon^2|t|^{-1} - \frac{\varepsilon^2}{4}\sup_{z\in I_{\varepsilon,t}} \tilde{J}^{-2}(z) - \frac{\varepsilon}{2}\big(\Psi_1(1/\varepsilon)\big)^2 \\ &\ge \lambda_1^0 - c_5\varepsilon^2|t|^{-1} - \varepsilon^2|t|^{-1} - c_7\varepsilon e^{-2\sqrt{2}/\varepsilon}\tilde{J}^{-1}(a_0') \ge -c_8\varepsilon^2|t|^{-1}, \end{aligned}$$

provided that ε is sufficiently small so that $e^{-2\sqrt{2}/\varepsilon}\tilde{J}^{-1}(a_0') \le \varepsilon$. □

Remark 3.1. For $t \le -\varepsilon^2 \log(\varepsilon^{-1})^2$ we have the upper bound $\lambda_1 \le c_6\varepsilon^2|t|^{-1}$.

4. Conclusion

We have discussed in this paper the robustness of error estimates for the approximation of phase field models with standard numerical techniques. Those error estimates avoid an explicit exponential dependence on the inverse of the small phase field parameter but include the principal eigenvalue of the linearized differential operator. The precise properties of this crucial quantity are only rigorously understood for the smooth evolution of interfaces. Numerical experiments reveal a scaling behavior at singularities that implies the robustness of the error estimates through topological changes. For an important class of generic topological changes we have shown that this behavior can be rigorously analyzed and thereby explained the surprisingly good approximation properties of standard computational methods at singularities.

Appendix A. Experimental verification of Assumption A

For a triangulation $\mathcal{T}$ of B_2 with mesh-size $h \sim 2^{-8}$ we approximated the Allen–Cahn problem with a semi-implicit time-stepping scheme with step-size $\tau = h/10$ for the initial data $u_0(r) = \tanh\big((r - \sqrt{2}|t_0|^{1/2})\big)/\varepsilon$ at $t_0 = -1/4$. In Fig. 2 we plotted for $\varepsilon = 2^{-\ell}$, $\ell = 2, 3, 4, 5$ the quantity

$$\eta_\varepsilon(t) := \varepsilon^{-2} \max_{z\in\mathcal{N}} |u_h(z,t) - \tanh\big((|z| - \sqrt{2}|t|^{1/2})/\varepsilon\big)|,$$

where $\mathcal{N}$ denotes the set of nodes in the triangulation $\mathcal{T}$. The results show that $\eta_\varepsilon(t) \le c|t|^{-1}$ and thus justify Assumption A.

Appendix B. Comparison principles

Lemma B.1. (a) *Let $a < b$, set $I := (a,b) \subseteq \mathbb{R}$, let $p, q \in C(I)$, and suppose $p \ge q \ge 0$. Assume $\Psi, \Phi \in C^2(\mathbb{R})$, satisfy $\Psi \ge 0$, $\Psi(a) = \Phi(a)$, $\Psi'(b) = \Phi'(b) = 0$, and*

$$-\Psi'' + p\Psi = 0, \qquad -\Phi'' + q\Phi = 0 \quad \text{in } I.$$

Then $\Psi \le \Phi$. The same conclusion holds if $\Psi(b) = \Phi(b)$ and $\Psi'(a) = \Phi'(a) = 0$.

(b) *Let $a < b$ set $I_+ := (a,b)$ and $I_- := (-b,-a)$. For $\psi \in C(\mathbb{R})$ and $c \ge 0$ the functions $\Phi_\pm : I_\pm \to \mathbb{R}$, defined by*

$$\Phi_\pm : z \mapsto \Psi(\pm a)\frac{\cosh(c(b \mp z))}{\cosh(c(b-a))}$$

satisfy $\Phi_\pm(\pm a) = \Psi(\pm a)$, $\Phi_\pm'(\pm b) = 0$, and $-\Phi_\pm'' + c^2\Phi_\pm = 0$ in $I_\pm$. For $z \in I_\pm$ we have

$$|\Phi_\pm(z)| \le 2|\Psi(\pm a)|e^{-c|z|}e^{ca}. \tag{B.1}$$

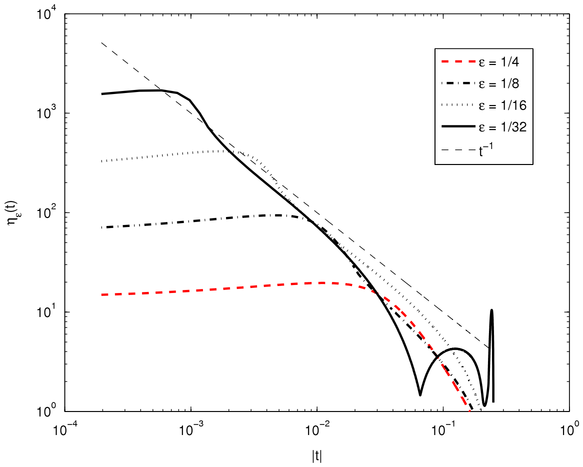

Fig. 2. Experimental bounds on the second order term in the asymptotic expansion.

Proof. (a) The function $E := \Psi - \Phi$ satisfies $E(a) = 0$, $E'(b) = 0$, and $-E'' + qE \le 0$ in I. Suppose there exist $a \le \alpha < \beta \le b$ such that $E|_{(\alpha,\beta)} > 0$ and $E(\alpha) = E(\beta) = 0$. Then $E'(\alpha) > 0$ and $E'(\beta) \le 0$ contradict $E'' \ge qE \ge 0$ in (α, β), i.e., the fact that E' is monotonically increasing in (α, β). Hence, $E \le 0$, i.e., $\Psi \le \Phi$. The second case is analogous.

(b) The identities follow from $\cosh'' = \cosh$ and $\sinh(0) = 0$. The estimates are consequences of the bounds

$$\frac{\cosh(c(b \mp z))}{\cosh(c(b-a))} = \frac{e^{c(b\mp z)} + e^{-c(b\mp z)}}{e^{c(b-a)} + e^{-c(b-a)}} = \frac{e^{\mp cz} e^{cb}}{e^{-ca} e^{cb}} \left(\frac{1 + e^{-2c(b\mp z)}}{1 + e^{-2c(b-a)}} \right) \le 2 e^{\mp cz} e^{ca}, \tag{B.2}$$

where we used $e^{-2c(b\mp z)} \le 1$ for $z < b$ and $-b < z$, respectively. □

Lemma B.2. *Let $a < b$ such that $I = (a, b) \subseteq I_{\varepsilon,t} := \big(-|t|^{1/2}/(\sqrt{2}\varepsilon), 1/\varepsilon\big)$, $p \in C(I)$, and $c \ge 0$ such that $p \ge c^2$. Let $\Psi \in C^2(I)$ be non-negative with $\Psi'(b) = 0$ and*

$$-\tilde{J}^{-1} \frac{d}{dz}\Big(\tilde{J} \frac{d}{dz}\Big) \Psi + p\Psi = 0$$

in I, where $\tilde{J}^{-1} = 1/\tilde{J}$ with $\tilde{J}(z) = \varepsilon z + \sqrt{2}|t|^{1/2}$. Then, $\Psi(z) \le 2\Psi(a) e^{-cz} e^{ca}$.

Proof. Defining

$$\Phi : I \to \mathbb{R}, \qquad z \mapsto \Psi(a) \frac{\cosh(c(b-z))}{\cosh(c(b-a))}$$

we have $-\Phi'' + c^2\Phi = 0$, $\Phi(a) = \Psi(a)$, and $\Phi'(b) = 0$. With $\tilde{J}_z = \varepsilon$ and $\Phi' \le 0$, $\tilde{J} > 0$ in I we deduce

$$-\tilde{J}^{-1} \frac{d}{dz}\Big(\tilde{J} \frac{d}{dz}\Big) \Phi + c^2\Phi = -\varepsilon \tilde{J}^{-1}\Phi' - \tilde{J}^{-1}\tilde{J}\Phi'' + c^2\Phi = -\varepsilon\tilde{J}^{-1}\Phi' \ge 0.$$

Since $p \ge c^2$ and $\Psi \ge 0$ the function $E := \Psi - \Phi$ satisfies

$$-\tilde{J}^{-1} \frac{d}{dz}\Big(\tilde{J} \frac{d}{dz}\Big) E + c^2 E = \varepsilon \tilde{J}^{-1}\Phi' \le 0$$

and $E(a) = 0$, $E'(b) = 0$. Suppose that $(\alpha, \beta) \subseteq I$ is maximal with $E|_{(\alpha,\beta)} > 0$. Then, since $\tilde{J} > 0$ we have $\tilde{J}(\alpha)E'(\alpha) > 0$ and $\tilde{J}(\beta)E'(\beta) \le 0$. This contradicts

$$\frac{d}{dz}(\tilde{J}E') = \frac{d}{dz}\Big(\tilde{J}\frac{d}{dz}\Big) E \ge \tilde{J} c^2 E \ge 0$$

and shows that $E \le 0$, i.e., $\Psi \le \Phi$. The proof of the estimate follows from (B.2). □

References

[1] Xiaobing Feng, Andreas Prohl, Numerical analysis of the Allen–Cahn equation and approximation for mean curvature flows, Numer. Math. 94 (1) (2003) 33–65.

[2] Daniel Kessler, Ricardo H. Nochetto, Alfred Schmidt, A posteriori error control for the Allen–Cahn problem: circumventing Gronwall's inequality, M2AN Math. Model. Numer. Anal. 38 (1) (2004) 129–142.

[3] Sören Bartels, A posteriori error analysis for time-dependent Ginzburg–Landau type equations, Numer. Math. 99 (4) (2005) 557–583.

[4] Sören Bartels, Rüdiger Müller, Christoph Ortner, Robust a priori and a posteriori error analysis for the approximation of Allen–Cahn and Ginzburg–Landau equations past topological changes, SIAM J. Numer. Anal. 49 (1) (2011) 110–134.

[5] Nicholas D. Alikakos, Giorgio Fusco, The spectrum of the Cahn–Hilliard operator for generic interface in higher space dimensions, Indiana Univ. Math. J. 42 (2) (1993) 637–674.

[6] Xinfu Chen, Spectrum for the Allen–Cahn, Cahn–Hilliard, and phase-field equations for generic interfaces, Comm. Partial Differential Equations 19 (7–8) (1994) 1371–1395.

[7] Piero de Mottoni, Michelle Schatzman, Geometrical evolution of developed interfaces, Trans. Amer. Math. Soc. 347 (5) (1995) 1533–1589.

[8] Tom Ilmanen, Convergence of the Allen–Cahn equation to Brakke's motion by mean curvature, J. Differential Geom. 38 (2) (1993) 417–461.

[9] Giovanni Bellettini, Maurizio Paolini, Quasi-optimal error estimates for the mean curvature flow with a forcing term, Differential Integral Equations 8 (4) (1995) 735–752.

[10] Maurizio Paolini, Claudio Verdi, Asymptotic and numerical analyses of the mean curvature flow with a space-dependent relaxation parameter, Asymptot. Anal. 5 (6) (1992) 553–574.

[11] Michael E. Gage, Richard S. Hamilton, The heat equation shrinking convex plane curves, J. Differential Geom. 23 (1) (1986) 69–96.

[12] David Gilbarg, Neil S. Trudinger, Elliptic Partial Differential Equations of Second Order, in: Classics in Mathematics, Springer-Verlag, Berlin, 2001, Reprint of the 1998 edition.