Error Controlled Local Resolution of Evolving Interfaces for Generalized Cahn-Hilliard Equations

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Abstract

For phase field equations of generalized Cahn-Hilliard type, we present an a posteriori error analysis that is robust with respect to a small interface length scale γ which enters the model as a regularizing parameter. By the solution of a fourth order elliptic eigenvalue problem in each time step we gain a fully computable error bound. In accordance with theoretical results, this error bound only depends on the inverse of the small parameter in a low order polynomial for a smooth evolution of the interface. We apply the general framework to the technologically relevant Cahn-Hilliard system coupled with homogeneous elasticity. The derived estimators can be used for adaptive mesh refinement and coarsening. In numerical examples we illustrate that the computation of the principal eigenvalue allows the detection of critical points during the time evolution like merging of interfaces or other topological changes. Moreover, it confirms theoretical predictions about fast relaxation of nonsmooth components in the initial data.

1 Introduction

Phase separation of an initially homogeneous mixture can be observed in many metal alloys and has influence on the quality and properties of the materials in technical applications [15, 8]. On a mesoscopic length scale, phase field models of Cahn-Hilliard-type serve as a general continuum model for these processes. They are often based on a minimization of the Ginzburg-Landau free energy functional

$$E(\rho,\vec{u}) := \int_\Omega \frac{\gamma^2}{2}\,|\nabla\rho|^2 + \mathcal{F}(\rho) + \mathcal{W}\left(\rho,\mathcal{E}(\vec{u})\right)\,\mathrm{d}x\,. \tag{1}$$

Here, the phase field variable $\rho(x)\in[-1,1]$ denotes the difference between the volume fractions of the two components in a binary alloy. Regions of pure phases are separated by diffuse interfaces that have a thickness of the order γ. $\mathcal{F}(\rho)$ is a *double well potential* that defines the stable states at $\rho=\pm1$. The influence of elastic stresses due to a lattice misfit is modeled by the term $\mathcal{W}\left(\rho,\mathcal{E}(\vec{u})\right)$, where the *displacement* $\vec{u}$ is a continuous function related to the mapping of the reference domain Ω to the volume actually occupied by the material. Assuming only small deformations, the *strain* is approximated by the symmetric gradient $\mathcal{E}(\vec{u}) := \frac{1}{2}(\nabla\vec{u}+\nabla\vec{u}^{\mathrm{T}})$. In the pure Cahn-Hilliard model elastic effects are neglected, but during the time evolution they become more and more important and will finally be the dominant influence [15]. The H^{-1} gradient flow of (1) leads to the fourth order semilinear parabolic equation

$$\partial_t\rho - \Delta\Big(-\gamma\Delta\rho + \frac{1}{\gamma}f(\rho) + \frac{1}{\gamma}W(\rho,\mathcal{E}(\vec{u}))\Big) = 0\,, \tag{2}$$

where $f(\rho) := \mathcal{F}'(\rho)$ and $W(\rho,\mathcal{E}(\vec{u})) = \partial_\rho\mathcal{W}(\rho,\mathcal{E}(\vec{u}))$. Because the time scale of mechanical relaxation is much smaller than the scale at which diffusion takes place, we may assume an equilibrium state governed by

$$0 = \operatorname{div}\left(\mathcal{C}\left[\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right]\right) \ \text{ in } \Omega\,. \tag{3}$$

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Here, $\mathcal{C}$ denotes the *elasticity tensor*. By $\bar{\mathcal{E}}(\rho) := \kappa \mathbb{I} \rho$ we denote the *stress free strain*, where $\mathbb{I}$ is the unit tensor and κ is called misfit.

The Cahn-Larché system consists of (2) and (3) together with initial and boundary conditions. In general, the elasticity tensor $\mathcal{C}$ may depend on ρ. It is called *homogeneous*, if $\mathcal{C}$ is independent of ρ. In this case there is a linear solution operator $\mathcal{D}^{-1}$ to (3), such that $\vec{u} = \mathcal{D}^{-1}\rho$ and we can write $W(\rho, \mathcal{E}(\vec{u})) =: A\rho$ with some linear operator A. This reduces (2) and (3) to the single equation

$$\partial_t \rho - \Delta\Big(-\gamma\Delta\rho + \frac{1}{\gamma} f(\rho) + \frac{1}{\gamma} A\rho\Big) = 0\,. \tag{4}$$

The error analysis presented in this paper is valid for Cahn-Hilliard type equations of the form (4), with a general linear selfadjoint operator A, that does not have to be related to elastic effects. On the other hand, the approximation scheme devised below in Section 6 is stated for the general Cahn-Larché system, that might not be of the form (4), e.g. if the elasticity tensor $\mathcal{C}$ is inhomogeneous.

Remark 1.1. a) The time scaling in (2) is chosen in such a way that topological changes of the solution take place during a fixed time period T that is independent of γ. In the limit $\gamma \to 0$ the Cahn-Hilliard model (i.e. $\mathcal{W} = 0$) converges to the Mullins-Sekerka model [1, 22].
b) There is no maximum principle for the Cahn-Hilliard equation (2) that would guarantee $\rho \in [-1, 1]$ for $T > 0$. Because the equation is in divergence form, total mass is conserved, i.e.

$$\bar{\rho}(t) := \frac{1}{|\Omega|}\int_\Omega \rho(t,x)\,\mathrm{d}x = \frac{1}{|\Omega|}\int_\Omega \rho_0(x)\,\mathrm{d}x =: \bar{\rho}_0\,.$$

c) Minimizing the same Ginzburg-Landau energy functional (1) with respect to the L^2 scalar product leads to the Allen-Cahn equation, a nonconservative second order equation, that obeys a maximum principle.
d) When natural boundary conditions $\vec{n} \cdot \big(\mathcal{C}\,[\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)]\big) = 0$ are prescribed on all of the domain boundary $\partial\Omega$, then $\vec{u}$ is not uniquely determined by the elasticity equation (3). From the solution space we have to exclude the kernel of $\mathcal{E}$, which contains all linearized rigid body motions; $W(\rho, \mathcal{E}(\vec{u}))$ depends only on $\mathcal{E}(\vec{u})$, not on $\vec{u}$ itself.

For a fixed size of the parameter γ the numerical analysis of the Cahn-Hilliard and Cahn-Larché equations is well established [10, 6, 24, 17]. When γ becomes small, the solution ρ is of low effective regularity and numerical approximation takes great advantage of mesh adaptivity. That in turn requires error control based on a posteriori estimates, but up to now, these error estimates depend exponentially on γ^{-1}, owing to an application of Gronwall's Lemma. For an a priori estimate, the dependence on the parameter γ^{-1} was reduced to a low order polynomial in [11, 12, 13]. A posteriori error estimates for the Allen-Cahn equation, that are robust with respect to the small parameter γ, have been presented in [18, 3]. These results are based on estimates for the principal eigenvalue of the linearized operator about the exact or the approximate solution. Transferring this idea to Cahn-Hilliard type equations, one looks for the largest number λ and a function $q \neq 0$ such that

$$\lambda\, q = \Delta\Big(-\gamma\Delta q + \frac{1}{\gamma} f'(\widehat{\rho}_h)\, q + \frac{1}{\gamma} A\, q\Big)\,.$$

Recent results in [14] provide an a posteriori error analysis for Cahn-Hilliard equations under the assumption that the principal eigenvalue defined through the exact solution remains bounded. This leads to restrictive assumptions on the initial data that we want to avoid. Instead, to guarantee the uniform boundedness of λ with respect to γ^{-1}, we propose to numerically approximate the principal eigenvalue $-\lambda$ in each time step and thereby measure the stability of the solution and detect critical points of the nonlinear evolution. The computation of the principal eigenvalue of the linearized operator about the discrete approximate solution is especially of great importance for Cahn-Larché system since in this case there is no spectral estimate available to get a bound of the principal eigenvalue. Moreover, our approach fits well into the methodology of a posteriori error estimation as it provides important information about the approximation. Our main result states that robust a posteriori error estimation is possible as long as an approximation of $-\lambda$ remains bounded from above in the time interval $[\gamma, T]$, cf. Theorem 3.4 and Remark 3.5 below.

As opposed to the work carried out for the Allen-Cahn equation, that is only of second order, we have to measure the error in the weaker H^{-1} norm. This makes it significantly harder to get control on the super-quadratic term in the error equation, so at least for space dimension $d = 3$ we have to impose a non-standard growth condition on the potential function $f(\rho)$. We remark that if a priori bounds are employed, then our error analysis could be modified to cover the case of more general potentials. This however is not in the spirit of a posteriori error estimation. In this fourth order problem, we have to take care of different constraints to the solution and the particular representation of the error defined below. For the eigenvalue problem, that is also of fourth order, we have to derive a computable a posteriori error bound and again, there are some constraints to the eigenfunctions to be taken into account.

The outline of this article is as follows. In the next section we introduce the finite element setting and the weak formulation of the considered problem, then we derive the error equation. The main result is stated in Section 3, where the aforementioned a posteriori error estimate is proven. In Section 4 we give an a posteriori upper bound for the numerically computed eigenvalue. To show that the assumptions are not too restrictive we complement this result by an a priori estimate. A finite element method for the Cahn-Larché system is given in Section 5 along with the corresponding residual estimators. Finally, in Section 6 we show the results of numerical experiments.

2 Problem Formulation and Finite Element Spaces

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded Lipschitz domain and $T > 0$ a time horizon. We use standard notation for Lebesgue and Sobolev spaces and denote the inner product of $L^2(\Omega)$ by (v, w). The duality pairing between a Banach space X and its dual X^* is written $\langle \cdot, \cdot \rangle$. We define

$$\bar{v} := \int_\Omega v \, \mathrm{d}x \,, \qquad \mathring{H}^1(\Omega) := \{v \in H^1(\Omega) : \bar{v} = 0\} \,.$$

The inverse Laplacian with natural boundary conditions $\Delta_N^{-1} : \mathring{H}^1(\Omega) \to \mathring{H}^1(\Omega)$ is defined by

$$\big(\nabla \Delta_N^{-1} v, \nabla \varphi\big) = -\,(v, \varphi) \qquad \text{for all } v \in \mathring{H}^1(\Omega) \text{ and } \varphi \in H^1(\Omega).$$

We restrict our analysis to continuous potential functions, of which the most common example is $\mathcal{F}^*(\rho) := (\rho^2 - 1)^2/4$. More realistic nonsmooth logarithmic potential functions have been proposed and quantitatively studied e.g. in [2, 6] but do not fit into our analysis. The following assumptions on the double well potential and the linear operator A are essential for our analysis:

(A1) $f \in C^1(\mathbb{R})$ and there is a constant $C_f \geq 0$ such that $-f' \leq C_f$.

(A2) There are a function g^* and constants $C_\delta \geq 0$ and $\delta \in (0, 1]$, with $\delta \leq 4/5$ if $d = 3$, such that for all $a, b \in \mathbb{R}$

$$-(b-a)\,(f(b) - f(a)) \leq -f'(b)(b-a)^2 + g^*(b)\, C_\delta \, |b-a|^{2+\delta} \,.$$

(A3) $A : L^2(\Omega) \to L^2(\Omega)$ is a bounded linear selfadjoint operator and there are constants $\alpha, C_A > 0$, such that

$$\begin{aligned} -\,(\varphi, A\,\varphi) &\leq \alpha \,\|\varphi\|_{L^2(\Omega)} && \text{for all } \varphi \in L^2(\Omega)\,, \\ (\psi, A\,\varphi) &\leq C_A \,\|\nabla\psi\|_{L^2(\Omega)} \,\|\nabla\varphi\|_{L^2(\Omega)} && \text{for all } \psi, \varphi \in \mathring{H}^1(\Omega)\,. \end{aligned}$$

Because there is no maximum principle available for the Cahn-Hilliard equation, the properties of f outside of $[-1, 1]$ may matter. Thus, if $d = 3$ we can not use $f^* := \mathcal{F}^{*\prime}$ given above on all of $\mathbb{R}$ since f^* fails to satisfy (A2). Nevertheless a proper modification of f^* outside of $[-1, 1]$ is possible or alternatively a suitable replacement for the free energy function may be used.

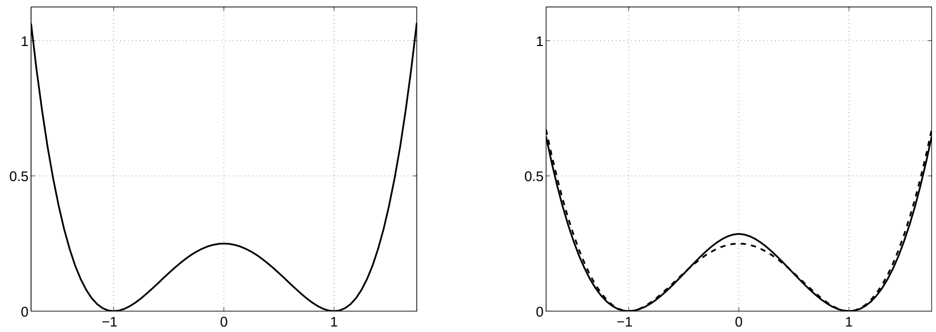

Figure 1: Left: quartic potential $\mathcal{F}^*$; right: alternative potentials: $\mathcal{F}_1$ and $\mathcal{F}_2$ (dashed).

Lemma 2.1. *a) Let $f^* = \mathcal{F}^{*\prime}$ for the quartic potential $\mathcal{F}^*$. If $d = 2$, f^* satisfies (A1) and (A2) with $g^*(b) = 3b$, $C_\delta = 1$ and $C_f = 1$.*
b) Let $0 < \delta \le 1$ and $f \in C^{1,\delta}(\mathbb{R})$, a continuously differentiable function with a Hölder continuous derivative with exponent δ respectively Lipschitz continuous derivative if $\delta = 1$. Then f satisfies assumption (A2).
c) Define

$$\mathcal{F}_1(x) := \frac{1}{2+\delta}|x|^{2+\delta} - \frac{1}{2}x^2 + \frac{\delta}{4+2\delta}\,, \qquad \mathcal{F}_2(x) := \begin{cases} \frac{2}{1+\delta}\left(\frac{1}{2+\delta}|x|^{2+\delta} + x\right) + \frac{2}{2+\delta} & \text{if } x < -1\,, \\ \frac{1}{4}x^4 - \frac{1}{2}x^2 + \frac{1}{4} & \text{if } |x| \le 1\,, \\ \frac{2}{1+\delta}\left(\frac{1}{2+\delta}|x|^{2+\delta} - x\right) + \frac{2}{2+\delta} & \text{if } x > 1\,. \end{cases}$$

Then $f_1(x) := \mathcal{F}_1'(x) = x|x|^\delta - x$ and $f_2(x) := \mathcal{F}_2'(x)$ satisfy assumptions (A1) and (A2).

Proof. a) Since $f(x) = x^3 - x$, we have the lower bound $f'(x) = 3x^2 - 1 \ge -1 =: -C_f$. Moreover, we note $f''(x) = 6x$. Then, for $a, b \in \mathbb{R}$, Taylor expansion yields

$$f(b) - f(a) = f'(b)(b-a) + f''(b)(b-a)^2/2 + f'''(b)(b-a)^3/6\,.$$

We multiply this identity $-(b-a)$ to verify

$$\begin{aligned} -(b-a)(f(b)-f(a)) &= -f'(b)(b-a)^2 - f''(b)(b-a)^3/2 - (b-a)^4 \\ &\le -f'(b)(b-a)^2 - 6b(b-a)^3/2\,. \end{aligned}$$

b) Let $a \ne b \in \mathbb{R}$ and $f \in C^{1,\delta}(\mathbb{R})$. By the meanvalue theorem $f(b) - f(a) = f'(\xi)(b-a)$ for some $\xi \in (\min(a,b), \max(a,b))$ and there is a constant C_δ such that

$$f'(\xi) - f'(b) \;\ge\; -|f'(\xi) - f'(b)| \;\ge\; -C_\delta|\xi - b|^\delta \;\ge\; -C_\delta|a-b|^\delta\,.$$

Thus the first assertion follows, when multiplying

$$\frac{f(b)-f(a)}{b-a} = f'(\xi) \ge f'(b) - C_\delta|b-a|^\delta$$

by $-(b-a)^2$. For c) we first note $f_1'(x) = (1+\delta)|x|^\delta - 1 \ge -1$ and then check $f_1 \in C^{1,\delta}(\mathbb{R})$: Without loss of generality assume $|a| \le |b|$, then

$$\begin{aligned} |f_1'(b) - f_1'(a)| &= (1+\delta)\left||b|^\delta - |a|^\delta\right| = (1+\delta)\left(|b|^\delta - |a|^\delta\right) \\ &\le (1+\delta)\left((|b-a| + |a|)^\delta - |a|^\delta\right) \le (1+\delta)\left(|b-a|^\delta + |a|^\delta - |a|^\delta\right) \\ &= (1+\delta)\,|b-a|^\delta\,, \end{aligned}$$

where in the last inequality, we used that for $\delta \le 1$ the mapping $x \mapsto x^\delta$ is concave. We easily verify that f_2 and f_2' are continuous at $x = \pm 1$. Moreover f_2' is Lipschitz continuous on $[-1,1]$, hence $|f_2'(b) - f_2'(a)| \le \widetilde{C}|b-a| = \widetilde{C}|b-a|^{1-\delta}\,|b-a|^\delta \le 2^{1-\delta}\widetilde{C}|b-a|^\delta =: C|b-a|^\delta$ for all $a, b \in [-1,1]$. By the same arguments as above, we see that f_2' is Hölder continuous with exponent δ on the intervals $(-\infty,-1]$ and $[1,\infty)$ and by triangle inequality we conclude, that $f_2 \in C^{1,\delta}(\mathbb{R})$. $\square$

Since we are interested in robust estimates for small γ we assume $0 < \gamma \leq 1$. To reduce the regularity requirements on the solution ρ, we introduce the *chemical potential* w defined as

$$w := -\gamma\Delta\rho + \gamma^{-1}\left(f(\rho) + A\,\rho\right)$$

and the solution space

$$X_{\mathrm{CH}} := \left(L^2\left([0,T], H^1(\Omega)\right) \cap H^1\left([0,T], H^1(\Omega)^*\right)\right) \times L^2\left([0,T], H^1(\Omega)\right) .$$

The mixed variational formulation of the Cahn-Hilliard type equation with natural boundary conditions reads as follows:

$$(\mathbf{P}) \quad \begin{cases} \text{Given } \rho(0,x) = \rho_0(x) \in H^1(\Omega), \text{ find} (\rho, w) \in X_{\mathrm{CH}} \text{ such that for almost all } t \in (0,T) \\ \langle \varphi, \partial_t \rho\rangle + (\nabla\varphi, \nabla w) = 0 \qquad \text{for all } \varphi \in H^1(\Omega)\,, \\ (\psi, w) - \gamma\,(\nabla\psi, \nabla\rho) = \gamma^{-1}\,(\psi, f(\rho) + A\,\rho) \qquad \text{for all } \psi \in H^1(\Omega)\,. \end{cases}$$

For the pure Cahn-Hilliard equation, i.e. for $A = 0$, the existence and uniqueness of a global solution to (P) has been established in [9, 10]. The existence of a solution to the Cahn-Larché system was proven in [16], together with a uniqueness result for the case of homogeneous elasticity.

The quantities ρ and w are discretized with lowest order conforming finite elements. We consider shape regular meshes $\mathcal{T}$ without hanging nodes, which consist of simplicial elements and define the $\mathcal{T}$-elementwise constant function $h_{\mathcal{T}} : \Omega \to \mathbb{R}$ by $h_{\mathcal{T}}|_K := \mathrm{diam}(K)$ for all $K \in \mathcal{T}$. The set of all element faces within $\mathcal{T}$ is denoted by $\mathcal{E}(\mathcal{T})$ and we assign to each $E \in \mathcal{E}(\mathcal{T})$ its diameter h_E. Then, we denote the skeleton $\{x \in \overline{\Omega} : x \in E, E \in \mathcal{E}(\mathcal{T})\}$ of $\mathcal{T}$ by $\bigcup\mathcal{E}(\mathcal{T})$ and introduce the function $h_{\mathcal{E}} \in L^\infty(\bigcup\mathcal{E}(\mathcal{T}))$ that satisfies $h_{\mathcal{E}}|_E = h_E$ for all $E \in \mathcal{E}$.

Let $0 = t_0 < t_1 < \ldots < t_M = T$ be a partition of the time interval $[0,T]$. At time step j the mesh is denoted by $\mathcal{T}^{(j)}$ and the approximation space is denoted by $\mathcal{S}(\mathcal{T}^{(j)})$. Often we abbreviate $\mathcal{E}^{(j)} := \mathcal{E}(\mathcal{T}^{(j)})$ and $\mathcal{S}^{(j)} := \mathcal{S}(\mathcal{T}^{(j)})$. On the subspace $\mathring{\mathcal{S}}^{(j)}$ of finite element functions having meanvalue zero, the discrete inverse Laplacian $\Delta_{Nh}^{-1} : \mathring{\mathcal{S}}^{(j)} \to \mathring{\mathcal{S}}^{(j)}$ satisfies

$$\left(\nabla\Delta_{Nh}^{-1} v_h, \nabla\varphi_h\right) = -\left(v_h, \varphi_h\right) \qquad \text{for all } v_h \in \mathring{\mathcal{S}}^{(j)} \text{ and } \varphi_h \in \mathcal{S}^{(j)}.$$

The operators $\Delta_{\mathcal{T}}$ and $\mathrm{div}_{\mathcal{T}}$ satisfy $\Delta_{\mathcal{T}}\varphi_h|_K = \Delta(\varphi_h|_K)$ for all $\varphi \in \mathcal{S}^{(j)}$ and $K \in \mathcal{T}$ and $\mathrm{div}_{\mathcal{T}}\,\vec{\xi}_h|_K = \mathrm{div}(\vec{\xi}_h|_K)$ for all $\mathcal{T}$-elementwise affine vector fields $\vec{\xi}$. To each face $E \in \mathcal{E}$ we assign a unique normal vector $\vec{n}$ and denote the neighboring elements $K^+, K^- \in \mathcal{T}$ in the way that $E = K^+ \cap K^-$ and the normal $\vec{n}$ points from K^+ to K^-. Then the jump operator is defined by $[\![\varphi]\!] := \varphi|_{K^+} - \varphi|_{K^-}$ for all $\mathcal{T}$-elementwise affine functions φ.

Definition 2.2. a) Let $(\rho, w) \in X_{CH}$ be the solution of (P) and (ρ_h, w_h) a conforming finite element approximation. For almost all $t \in [0,T]$, we define the *errors*

$$\bar{e}_1 := \bar{\rho}_h - \bar{\rho}_0 \in \mathbb{R}\,, \quad \mathring{e}_1 := \rho_h - \rho - \bar{e}_1 \in \mathring{H}^1(\Omega)\,, \quad e_2 := w_h - w \in H^1(\Omega)\,.$$

We set

$$\widehat{\rho}_h := \rho_h - \bar{e}_1\,, \qquad z := -\Delta_N^{-1}\mathring{e}_1.$$

b) For $s \in (0,T)$ the *residuals* $R_1(s)$, $R_2(s) \in H^1(\Omega)^*$ of the approximation (ρ_h, w_h) are defined as

$$\langle\varphi, R_1\rangle := (\nabla\varphi, \nabla w_h) + \langle\varphi, \partial_t\rho_h\rangle \qquad \text{for all } \varphi \in H^1(\Omega)\,, \tag{5a}$$

$$\langle\psi, R_2\rangle := \gamma\,(\nabla\psi, \nabla\rho_h) - (\psi, w_h) + \gamma^{-1}\,(\psi, f(\rho_h) + A\,\rho_h) \qquad \text{for all } \psi \in H^1(\Omega)\,. \tag{5b}$$

Remark 2.3. If $\bar{\rho}_h^{(0)} = \bar{\rho}_0$ and a fixed triangulation $\mathcal{T}^{(j)} = \mathcal{T}^{(0)}$ for $j = 1, 2, \cdots M$ is used, or if $\mathcal{T}^{(j)}$ is a refinement of $\mathcal{T}^{(j-1)}$ for all $j \geq 0$, then $\bar{e}_1 = 0$.

We note that if the finite element solution coincides with the exact solution then the residuals vanish. In order to derive an error equation, we choose $\varphi = z$ in (5a), set $\psi = \mathring{e}_1$ in (5b) and subtract the weak formulation from the definition of the residuals, i.e.

$$\langle z, R_1\rangle = (\nabla z, \nabla e_2) + \langle z, \partial_t \mathring{e}_1\rangle + \langle z, \partial_t \bar{\rho}_h\rangle \ , \tag{6a}$$

$$\langle \mathring{e}_1, R_2\rangle = \gamma \left\|\nabla \mathring{e}_1\right\|^2_{L^2(\Omega)} - (\mathring{e}_1, e_2) + \frac{1}{\gamma}\left(\mathring{e}_1, f(\rho_h) - f(\rho) + A\,\rho_h - A\,\rho\right) \ . \tag{6b}$$

Note $\langle z, \partial_t \mathring{e}_1\rangle = -\langle z, \partial_t \Delta z\rangle = \langle \nabla z, \partial_t \nabla z\rangle = \frac{1}{2}\frac{d}{dt}\left\|\nabla z\right\|^2_{L^2(\Omega)}$ and $(z, \partial_t \bar{\rho}_h) = 0$ because $z \in \mathring{H}^1(\Omega)$. By definition of z we have $(\mathring{e}_1, e_2) = (\nabla z, \nabla e_2)$. Thus, when adding (6a) and (6b), the mixed terms cancel and we obtain the identity

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|\nabla z\right\|^2_{L^2(\Omega)} + \gamma\left\|\nabla \mathring{e}_1\right\|^2_{L^2(\Omega)} &= \langle z, R_1\rangle + \langle \mathring{e}_1, R_2\rangle - \gamma^{-1}\left(\mathring{e}_1, A\,\bar{e}_1\right)\\ &\quad - \gamma^{-1}\left(\mathring{e}_1, f(\rho_h) - f(\rho) + A\,\mathring{e}_1\right) \ .\end{aligned} \tag{7}$$

Because of $\mathring{e}_1 \in \mathring{H}^1(\Omega)$, by Poincaré's inequality there is a constant C_P, depending only on Ω, such that $\left\|\mathring{e}_1\right\|_{L^2(\Omega)} \leq C_P\left\|\nabla \mathring{e}_1\right\|_{L^2(\Omega)}$. Instead of using this, we will sometimes apply Young's inequality with a positive factor $\varepsilon > 0$ to insert appropriate powers of γ:

$$\left\|\mathring{e}_1\right\|^2_{L^2(\Omega)} = (\nabla \mathring{e}_1, \nabla z) \ \leq \varepsilon\left\|\nabla \mathring{e}_1\right\|^2_{L^2(\Omega)} + \frac{1}{4\varepsilon}\left\|\nabla z\right\|^2_{L^2(\Omega)} \ . \tag{8}$$

3 A posteriori Error Estimate

Our main result relies on an application of Gronwall's Lemma to (7). Therefore we have to get appropriate bounds on the nonlinear contribution to the right-hand side. To estimate the nonlinear potential f, we consider the smallest eigenvalue of the linearized operator about the corrected discrete approximation $\widehat{\rho}_h$,

$$-\lambda(s) := \inf_{\substack{q\in \mathring{H}^1(\Omega)\setminus\{0\}\\ y=-\Delta_N^{-1}q}} \frac{\gamma\left\|\nabla q\right\|^2_{L^2(\Omega)} + \gamma^{-1}\left(q, f'(\widehat{\rho}_h(s))q\right) + \gamma^{-1}\left(q, Aq\right)}{\left\|\nabla y\right\|^2_{L^2(\Omega)}} \ . \tag{9}$$

When $A = 0$, i.e. in case of the Cahn-Hilliard problem, it is known, that if ρ describes bulk phase regions separated by transition zones of width $O(\gamma)$, then $-\lambda$ is uniformly bounded from below with respect to γ^{-1}, as long as no topological changes occur [5, 7]. Instead of assuming a priori bounds on the spectrum of the linearized operator, we use a numerically computed eigenvalue Λ and the a posteriori estimate of Theorem 4.4 to define

$$-\Lambda^* := \inf_{s\in[0,T]}(-\Lambda - \eta_\Lambda) \leq \inf_{s\in[0,T]} -\lambda \, . \tag{10}$$

Lemma 3.1. *Let $-\Lambda^*$ be a lower bound for the principal eigenvalue $-\lambda$ in (9) and define $\eta_f := \left\|f(\rho_h) - f(\widehat{\rho}_h)\right\|_{L^2(\Omega)}$, $\widetilde{\eta}_{g^*} := \left\|g^*(\rho_h)\right\|_{L^\infty(\Omega)}$. The assumptions (A1), (A2) and (A3) imply*

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|\nabla z\right\|^2_{L^2(\Omega)} + \frac{3}{4}\gamma\left\|\nabla \mathring{e}_1\right\|^2_{L^2(\Omega)} &\leq \langle z, R_1\rangle + \langle \mathring{e}_1, R_2\rangle - \gamma^{-1}\left(\mathring{e}_1, A\,\bar{e}_1\right) + \frac{1}{4\gamma}\eta_f^2\\ &\quad + \frac{(C_f + \alpha + 1)^2}{\gamma^3}\left\|\nabla z\right\|^2_{L^2(\Omega)} \ ,\end{aligned} \tag{11}$$

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|\nabla z\right\|^2_{L^2(\Omega)} &\leq \langle z, R_1\rangle + \langle \mathring{e}_1, R_2\rangle - \gamma^{-1}\left(\mathring{e}_1, A\,\bar{e}_1\right) + \frac{C_P^2}{\gamma^6}\eta_f^2\\ &\quad + \Lambda^*\left\|\nabla z\right\|^2_{L^2(\Omega)} + \widetilde{\eta}_{g^*}\frac{C_\delta}{\gamma}\left\|\mathring{e}_1\right\|^{2+\delta}_{L^{2+\delta}(\Omega)} + \frac{\gamma^4}{4(1-\gamma^3)}\left\|\nabla \mathring{e}_1\right\|^2_{L^2(\Omega)} \ .\end{aligned} \tag{12}$$

Proof. Because $\mathring{e}_1 = \widehat{\rho}_h - \rho$, we insert $f(\widehat{\rho}_h)$ to the terms in (7) containing the nonlinear potential

$$\begin{aligned}-\gamma^{-1}\left(\mathring{e}_1, f(\rho_h) - f(\rho)\right) &= -\gamma^{-1}\left(\mathring{e}_1, f(\widehat{\rho}_h) - f(\rho)\right) \ - \gamma^{-1}\left(\mathring{e}_1, f(\rho_h) - f(\widehat{\rho}_h)\right)\\ &\leq -\gamma^{-1}\left(\mathring{e}_1, f(\widehat{\rho}_h) - f(\rho)\right) \ + \gamma^{-1}\eta_f\left\|\mathring{e}_1\right\|_{L^2(\Omega)} \ .\end{aligned} \tag{13}$$

For the first assertion, from the fundamental theorem of calculus and assumption (A1) we get

$$-\gamma^{-1}\mathring{e}_1\,[f(\widehat{\rho}_h)-f(\rho)] = \gamma^{-1}\mathring{e}_1\int_{\rho}^{\widehat{\rho}_h} -f'(\xi)\,d\xi \quad \le \gamma^{-1}C_f\,\mathring{e}_1^2\,.$$

Integrating this identity over Ω and using (A3) and (13) where we apply Young's inequality to the last term containing η_f, we deduce

$$\begin{aligned}-\gamma^{-1}\left(\mathring{e}_1, f(\rho_h)-f(\rho)+A\mathring{e}_1\right) \le& \gamma^{-1}C_f\,\|\mathring{e}_1\|^2_{L^2(\Omega)} + \gamma^{-1}(1+\alpha)\,\|\mathring{e}_1\|^2_{L^2(\Omega)} + \frac{1}{4\gamma}\eta_f^2\,,\\ \le& \frac{1}{4}\gamma\,\|\nabla\mathring{e}_1\|^2_{L^2(\Omega)} + \frac{(C_f+\alpha+1)^2}{\gamma^3}\,\|\nabla z\|^2_{L^2(\Omega)} + \frac{1}{4\gamma}\eta_f^2\,.\end{aligned}$$

because of (8) with $\varepsilon = \gamma^2/4(C_f+\alpha+1)$. Inserting this into (7) proves the first assertion. To prove the second assertion, by assumption (A2) we get

$$\begin{aligned}-\gamma^{-1}\left[\,(\mathring{e}_1, f(\widehat{\rho}_h)-f(\rho)+A\,\mathring{e}_1)\,\right] \le& -\gamma^{-1}\left[\,(\mathring{e}_1, f'(\widehat{\rho}_h)\mathring{e}_1) + (\mathring{e}_1, A\,\mathring{e}_1)\,\right] + \widetilde{\eta}_{g^*}\frac{C_\delta}{\gamma}\,\|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)}\\ \le& \Lambda^*\,\|\nabla z\|^2_{L^2(\Omega)} + \gamma\,\|\nabla\mathring{e}_1\|^2_{L^2(\Omega)} + \widetilde{\eta}_{g^*}\frac{C_\delta}{\gamma}\,\|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)}\,, \qquad (14)\end{aligned}$$

owing to $-\Lambda^* \le -\lambda$ and (9), where we set $q = \mathring{e}_1 \in \mathring{H}^1(\Omega)$ in (9) and thus by definition $y = z$. Next, we again apply (13), but since we now want to avoid a term $\|\nabla z\|^2_{L^2(\Omega)}$ multiplied by a negative power of γ, we have to treat the term $\gamma^{-1}\eta_f\,\|\mathring{e}_1\|_{L^2(\Omega)}$ differently. We apply Young's and Poincaré's inequality to verify

$$\gamma^{-1}\left(\mathring{e}_1, f(\rho_h)-f(\widehat{\rho}_h)\right) \le \gamma^{-1}\,\eta_f\,\|\mathring{e}_1\|_{L^2(\Omega)} \le \frac{C_P^2(1-\gamma^3)}{\gamma^6}\eta_f^2 + \frac{\gamma^4}{4C_P^2(1-\gamma^3)}\,\|\mathring{e}_1\|^2_{L^2(\Omega)}\,.$$

A combination with (14) and $\gamma \le 1$ yield (12). □

The "coarse estimate" (11) is not sufficient for a robust error estimate, since an application of Gronwall's Lemma would lead to an error bound that depends exponentially on γ^{-1}. On the other hand, with the "fine estimate" (12) alone, we loose necessary control on the error $\|\nabla\mathring{e}_1\|_{L^2(\Omega)}$. In the following lemma both approaches are combined. The residual estimators involved in this lemma depend on the specific discretization scheme used. When A is given by linear elasticity, i.e. the elasticity tensor is homogeneous, we derive in Section 5 computable estimates of the residuals R_1 and R_2 that meet the stated requirements.

Lemma 3.2. *Assume there are computable estimators η_1, η_{21} and η_{22}, such that for almost every $t \in [0,T]$ and $\varphi, \psi \in \mathring{H}^1(\Omega)$*

$$\langle\varphi, R_1\rangle \le \eta_1\,\|\nabla\varphi\|_{L^2(\Omega)}\,, \quad \langle\psi, R_2\rangle \le \eta_{21}\,\|\nabla\psi\|_{L^2(\Omega)} + \eta_{22}\,\|\psi\|_{L^2(\Omega)}\,,$$

and define

$$\begin{aligned}\bar{\eta}_A^2 &:= \|A\,\bar{e}_1\|^2_{L^2(\Omega)}\\ \eta^2 &:= \frac{1}{4}\eta_1^2 + \frac{2}{\gamma^4}\eta_{21}^2 + \frac{4}{\gamma^2}\eta_{22}^2 + \left(\frac{\gamma^2}{4}+\frac{C_P^2}{\gamma^6}\right)\eta_f^2 + \frac{4}{\gamma^4}\bar{\eta}_A^2\,,\\ \Lambda_\circ &:= 1 + \frac{1}{32} + (C_f+\alpha+1)^2\,.\end{aligned}$$

Then, if $-\Lambda^*$ is a lower bound for the principal eigenvalue in (9) *we have*

$$\frac{1}{2}\frac{d}{dt}\,\|\nabla z\|^2_{L^2(\Omega)} + \frac{\gamma^4}{4}\,\|\nabla\mathring{e}_1\|^2_{L^2(\Omega)} \le \eta^2 + (\Lambda_\circ+\Lambda^*)\,\|\nabla z\|^2_{L^2(\Omega)} + \widetilde{\eta}_{g^*}\frac{C_\delta}{\gamma}\,\|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)}\,. \qquad (15)$$

Proof. Taking a convex combination of γ^3 times (11) plus $\left(1-\gamma^3\right)$ times (12) yields

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|\nabla z\right\|^2_{L^2(\Omega)}+\frac{1}{2}\gamma^4\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)} &\le \langle z,R_1\rangle+\langle\mathring{e}_1,R_2\rangle-\gamma^{-1}\left(\mathring{e}_1,A\,\bar{e}_1\right)\\ &\quad+\left((C_f+\alpha+1)^2+(1-\gamma^3)\Lambda^*\right)\left\|\nabla z\right\|^2_{L^2(\Omega)}\\ &\quad+\frac{\left(1-\gamma^3\right)C_\delta}{\gamma}\left\|\mathring{e}_1\right\|^{2+\delta}_{L^{2+\delta}(\Omega)}+\left(\frac{\gamma^2}{4}+\frac{C_P^2(1-\gamma^3)^2}{\gamma^6}\right)\eta_f^2\,.\end{aligned}$$

By Hölder's and Young's inequalities $-\frac{1}{\gamma}\left(\mathring{e}_1,A\,\bar{e}_1\right)\le\frac{1}{4\varepsilon_0\gamma^4}\bar{\eta}_A^2+\varepsilon_0\gamma^2\left\|\mathring{e}_1\right\|^2_{L^2(\Omega)}$ with some $\varepsilon_0>0$ and applying (8) with $\varepsilon=\gamma^2$, we have

$$-\frac{1}{\gamma}\left(\mathring{e}_1,A\,\bar{e}_1\right)\le\frac{1}{4\varepsilon_0\gamma^4}\bar{\eta}_A^2+\varepsilon_0\gamma^4\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}+\frac{\varepsilon_0}{4}\left\|\nabla z\right\|^2_{L^2(\Omega)}\,.$$

In the same way, we treat the residuals R_1 and R_2 to verify

$$\begin{aligned}\langle z,R_1\rangle+\langle\mathring{e}_1,R_2\rangle &\le \frac{1}{4}\eta_1^2+\left\|\nabla z\right\|^2_{L^2(\Omega)}+\frac{1}{4\varepsilon_{21}\gamma^4}\eta_{21}^2+\varepsilon_{21}\gamma^4\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}\\ &\quad+\frac{1}{4\varepsilon_{22}\gamma^2}\eta_{22}^2+\varepsilon_{22}\gamma^4\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}+\frac{\varepsilon_{22}}{4}\left\|\nabla z\right\|^2_{L^2(\Omega)}\,.\end{aligned}$$

On combining the last three estimates and choosing $\varepsilon_{21}=1/8$, $\varepsilon_0=\varepsilon_{22}=1/16$, we can absorb $(\varepsilon_0+\varepsilon_{21}+\varepsilon_{22})\gamma^4\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}=(\gamma^4/4)\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}$ on the left-hand side. □

The following (multiplicative) Sobolev inequalities are taken from [19].

Lemma 3.3. *a) Let $d=2$ and $\delta=1$. Then there is a constant $C_{S,\delta}>0$ such that*

$$\left\|v\right\|^2_{L^4(\Omega)}\le C_{S,\delta}\left\|v\right\|_{L^2(\Omega)}\left\|\nabla v\right\|_{L^2(\Omega)}\qquad\textit{for all } v\in\mathring{H}^1(\Omega)\,. \tag{16}$$

b) Let $d=2$ and $0\le\delta<1$. Then there is a constant $C_{S,\delta}>0$ such that

$$\left\|v\right\|_{L^{\frac{2-\delta}{1-\delta}}(\Omega)}\le C_{S,\delta}\left\|\nabla v\right\|_{L^2(\Omega)}\qquad\textit{for all } v\in\mathring{H}^1(\Omega)\,. \tag{17}$$

c) Let $d=3$ and assume $0\le\delta\le\frac{4}{5}$. Then there is a constant $C_{S,\delta}>0$ such that (17) is satisfied.

The continuation argument in the proof of the following theorem is adopted from [18].

Theorem 3.4. *Suppose $\Lambda_\circ$, Λ^* and the residual estimate η be given according to Lemma 3.2 and let $C_{S,\delta}$ be as in Lemma 3.3. Set $\eta_{g^*}:=\max(1,\sup_{t\in[0,T]}\widetilde{\eta}_{g^*})$ and*

$$\mu_1^2:=\left(\frac{e^{-2\max(0,\Lambda_\circ+\Lambda^*)T}}{16\,\eta_{g^*}\,C_\delta\,C_{S,\delta}^{2-\delta}}\right)^{1/\delta}\qquad\textit{and}\qquad\mu_2^2:=\min\left(\frac{3\,e^{-2\max(0,\Lambda_\circ+\Lambda^*)T}}{16},1\right)\,.$$

Given a tolerance $\theta\le\gamma^{5/\delta}\mu_1^2$, suppose the approximation error of the initial values and the residual estimate can be controlled by this tolerance θ in the sense that

$$\left\|\nabla z_0\right\|_{L^2(\Omega)}+\sqrt{2}\left\|\eta\right\|_{L^2([0,T])}\;<\;\mu_2\,\theta\;\le\;\mu_1^2\,\mu_2\,\gamma^{5/\delta}\,, \tag{18}$$

where $z_0:=z(0)=\Delta_N^{-1}(\rho_h^{(0)}-\rho_0-(\bar{\rho}_h^{(0)}-\bar{\rho}_0))$. Then, we have

$$\sup_{s\in[0,T]}\left\|\nabla z(s)\right\|^2_{L^2(\Omega)}+\frac{1}{2}\gamma^4\int_0^T\left\|\nabla\mathring{e}_1\right\|^2_{L^2(\Omega)}\,ds\le\theta^2\,.$$

Proof. We define the temporal interval

$$I_\theta := \left\{ t \in [0,T] : \Gamma(t) := \sup_{s\in(0,t)} \|\nabla z(s)\|^2_{L^2(\Omega)} + \frac{1}{2}\gamma^4 \int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ds \le \theta^2 \right\}. \tag{19}$$

Then, since $\|\nabla z_0\|_{L^2(\Omega)} < \theta$ the interval I_θ is nonempty and because $\Gamma(t)$ is continuous, I_θ is closed. To establish $I_\theta = [0,T]$ we need to show that I_θ also is relatively open in $[0,T]$. Let $t \in I_\theta$, then by definition of I_θ we have $\|\nabla z(t)\|_{L^2(\Omega)} \le \theta$, as well as

$$\int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ds \le 2\gamma^{-4}\theta^2 \, . \tag{20}$$

We integrate the estimate (15) in time over $[0,t]$ to verify

$$\begin{aligned}\|\nabla z(t)\|^2_{L^2(\Omega)} + \frac{1}{2}\gamma^4 \int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ds &\le 2(\Lambda_\circ + \Lambda^*) \int_0^t \|\nabla z\|^2_{L^2(\Omega)} \, ds \\ &\quad + \|\nabla z_0\|^2_{L^2(\Omega)} + 2\int_0^t \eta^2 \, ds + \eta_{g^*} \frac{2C_\delta}{\gamma} \int_0^t \|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)} \, ds \, .\end{aligned}$$

By assumption (18) we have $\|\nabla z_0\|^2_{L^2(\Omega)} + 2\int_0^T \eta^2 \, ds \le \left(\|\nabla z_0\|_{L^2(\Omega)} + \sqrt{2}\, \|\eta\|_{L^2([0,T])} \right)^2 \le (\mu_2\theta)^2$, so we deduce

$$\begin{aligned}\|\nabla z(t)\|^2_{L^2(\Omega)} + \frac{1}{2}\gamma^4 \int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ds &\le 2\max(0, \Lambda_\circ + \Lambda^*) \int_0^t \|\nabla z\|^2_{L^2(\Omega)} \, ds \\ &\quad + \mu_2^2\theta^2 + \eta_{g^*} \frac{2C_\delta}{\gamma} \int_0^t \|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)} \, ds \, .\end{aligned} \tag{21}$$

We aim at estimating $\|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)}$ in terms of $\|\nabla z\|_{L^2(\Omega)}$ and $\|\nabla \mathring{e}_1\|^2_{L^2(\Omega)}$. If $\delta < 1$, Hölder's inequality with exponents $1/\delta$ and $1/(1-\delta)$ implies

$$\int_\Omega |\mathring{e}_1|^{2+\delta} \, \mathrm{d}x \le \left\| |\mathring{e}_1|^{2\delta} \right\|_{L^{\frac{1}{\delta}}(\Omega)} \left\| |\mathring{e}_1|^{2-\delta} \right\|_{L^{\frac{1}{1-\delta}}(\Omega)} = \|\mathring{e}_1\|^{2\delta}_{L^2(\Omega)} \|\mathring{e}_1\|^{2-\delta}_{L^{\frac{2-\delta}{1-\delta}}(\Omega)} \tag{22}$$

and by Lemma 3.3 b) or c) as well as $\|\mathring{e}_1\|^{2\delta}_{L^2(\Omega)} \le \|\nabla \mathring{e}_1\|^{\delta}_{L^2(\Omega)} \|\nabla z\|^{\delta}_{L^2(\Omega)}$ we conclude

$$\int_\Omega |\mathring{e}_1|^{2+\delta} \, \mathrm{d}x \le \|\mathring{e}_1\|^{2\delta}_{L^2(\Omega)} \left(C_{S,\delta} \|\nabla \mathring{e}_1\|_{L^2(\Omega)} \right)^{2-\delta} \le C_S^{2-\delta} \|\nabla z\|^{\delta}_{L^2(\Omega)} \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, .$$

If $d = 2$ and $\delta = 1$ we deduce with Hölder's inequality and Lemma 3.3 a) that

$$\begin{aligned}\int_\Omega |\mathring{e}_1|^3 \, \mathrm{d}x &\le \|\mathring{e}_1\|_{L^2(\Omega)} \|\mathring{e}_1\|^2_{L^4(\Omega)} \\ &\le \|\mathring{e}_1\|_{L^2(\Omega)} \, C_{S,\delta} \|\mathring{e}_1\|_{L^2(\Omega)} \|\nabla \mathring{e}_1\|_{L^2(\Omega)} \\ &\le C_{S,\delta}^{2-\delta} \|\nabla z\|^{\delta}_{L^2(\Omega)} \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ,\end{aligned}$$

where in the last line we used $\|\mathring{e}_1\|^2_{L^2(\Omega)} = (\nabla z, \nabla \mathring{e}_1) \le \|\nabla z\|_{L^2(\Omega)} \|\nabla \mathring{e}_1\|_{L^2(\Omega)}$. In either case we can continue in the same way and incorporating (20) shows

$$\begin{aligned}\frac{2C_\delta}{\gamma} \int_0^t \|\mathring{e}_1\|^{2+\delta}_{L^{2+\delta}(\Omega)} \, ds &\le \frac{2\,\eta_{g^*}\, C_\delta\, C_{S,\delta}^{2-\delta}}{\gamma} \theta^\delta \int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)} \, ds \\ &\le \frac{4\,\eta_{g^*}\, C_\delta\, C_{S,\delta}^{2-\delta}\, \theta^\delta}{\gamma^5} \theta^2 \\ &\le 4\,\eta_{g^*}\, C_\delta\, C_{S,\delta}^{2-\delta} \left(\frac{\theta}{\gamma^{5/\delta}} \right)^\delta \theta^2 \quad \le 4\,\eta_{g^*}\, C_\delta\, C_{S,\delta}^{2-\delta}\, \mu_1^{2\delta}\, \theta^2 \, .\end{aligned}$$

We return to (21) and are now in the position to apply Gronwall's Lemma in such a way, that the resulting exponent $2\max(0,\Lambda_\circ+\Lambda^*)T$ is independent of γ^{-1}. We finally conclude

$$\begin{aligned}\|\nabla z(t)\|^2_{L^2(\Omega)} + \frac{1}{2}\gamma^4\int_0^t \|\nabla \mathring{e}_1\|^2_{L^2(\Omega)}\, ds &\le \left[\left(\mu_2^2 + 4\,\eta_{g^*}\,C_\delta\,C_{S,\delta}^{2-\delta}\,\mu_1^{2\delta}\right)\theta^2\right] e^{2\max(0,\Lambda_\circ+\Lambda^*)T} \\ &\le \left[\frac{3}{16}+\frac{1}{4}\right]\theta^2 \qquad < \frac{1}{2}\theta^2\,.\end{aligned}$$

Hence $\Gamma(t) < \theta^2$ and I_θ is also open. Altogether we have proved $I_\theta = [0,T]$. □

Remark 3.5. a) The theorem above guarantees error bounds that do not depend exponentially on γ^{-1} provided that Λ^* is independent of γ^{-1} or $T \le \gamma$. For the latter case we notice that $\Lambda \le \gamma^{-1}$, cf. (32) below.
b) From (18) we see that the minimal polynomial degree, in which the error estimate depends on γ^{-1} is 5, that is $d=2$ and $\delta = 1$. If $d=3$, due to the requirement $\delta \le 4/5$ the minimal polynomial degree is limited by $5/\delta > 6$.

4 Estimates for the Eigenvalue Approximation

In this section we derive a version of estimate (10) following ideas for the a posteriori error estimation of eigenvalue problems in [20]. The principal eigenvalue $-\lambda$ defined in (9) is well defined since, possibly after a constant shift, the nominator on the right-hand side is a strictly convex functional. Hence there is a minimizing $q \in \mathring{H}^1(\Omega)\setminus\{0\}$ with

$$\lambda\left(v, \Delta_N^{-1} q\right) = \gamma\,(\nabla v, \nabla q) + \gamma^{-1}\,(v, f'(\widehat{\rho}_h) q) + \gamma^{-1}\,(v, Aq) \qquad \text{for all } v \in \mathring{H}^1(\Omega). \tag{23}$$

In the discrete eigenvalue problem, we are looking for the smallest number $-\Lambda$ and a function $q_h \in \mathring{\mathcal{S}}\setminus\{0\}$ such that

$$\Lambda\left(v_h, \Delta_{Nh}^{-1} q_h\right) = \gamma\,(\nabla v_h, \nabla q_h) + \gamma^{-1}\,(v_h, f'(\widehat{\rho}_h) q_h) + \gamma^{-1}\,(v_h, A_h q_h) \qquad \text{for all } v_h \in \mathring{\mathcal{S}}\,. \tag{24}$$

Here, Δ_N^{-1} and A are replaced by approximations Δ_{Nh}^{-1} and A_h, respectively. If A is related to linear elasticity, an estimator η_A for the residual $(A_h - A)q_h$ is given in Lemma 5.3 below. Keeping the definition $y := -\Delta_N^{-1} q_h$ in mind, the proof of the following lemma can be directly transferred from standard a posteriori estimates for the Laplace equation.

Lemma 4.1 ([23])**.** *Let C_{Cl} be the constant related to estimates for the Clément interpolation operator and define the residual estimator*

$$\eta_{Nh} := C_{Cl}\left\|h_{\mathcal{T}}\left(\Delta_{\mathcal{T}}\Delta_{Nh}^{-1} q_h - q_h\right)\right\|_{L^2(\Omega)} + C_{Cl}\left\|h_{\mathcal{E}}^{1/2}[\![\partial_{\vec{n}}\Delta_{Nh}^{-1} q_h]\!]\right\|_{L^2(\cup\mathcal{E})}\,.$$

Then we have

$$\left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|_{L^2(\Omega)} \le \eta_{Nh} \qquad \textit{for all } q_h \in \mathring{\mathcal{S}}\,.$$

In the same way, we also get a lower bound of the form $\eta_{Nh} \le C\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\|_{L^2(\Omega)}$, where no oscillation terms appears because $q_h \in \mathring{\mathcal{S}}$. Hence, with the standard a priori estimates for the Laplace equation, we can always guarantee sufficient smallness of η_{Nh} for small mesh width h.

Definition 4.2. Given $(\Lambda, q_h) \in \mathbb{R}\times\mathring{\mathcal{S}}\setminus\{0\}$ satisfying (24), the *residual* R_Λ is defined by

$$\langle v, R_\Lambda\rangle := \Lambda\left(v, \Delta_N^{-1} q_h\right) - \gamma\,(\nabla v, \nabla q_h) - \gamma^{-1}\,(v, f'(\widehat{\rho}_h) q_h) - \gamma^{-1}\,(v, A\,q_h) \quad \text{for all } v \in \mathring{H}^1(\Omega)\,.$$

Lemma 4.3. *Let $(\Lambda, q_h) \in \mathbb{R}\times\mathring{\mathcal{S}}\setminus\{0\}$ be a solution of (24) and define the residual estimator*

$$\eta_{q_h} := C_{Cl}\left\|h_{\mathcal{T}}\left(\gamma\Delta_{\mathcal{T}} q_h + \gamma^{-1}(f'(\widehat{\rho}_h) q_h + A_h q_h) - \Lambda\,\Delta_{Nh}^{-1} q_h\right)\right\|_{L^2(\Omega)} + C_{Cl}\left\|h_{\mathcal{E}}^{1/2}\gamma[\![\partial_{\vec{n}} q_h]\!]\right\|_{L^2(\cup\mathcal{E})}\,,$$

with the constant C_{Cl} related to estimates for the Clément interpolation operator. If there is an estimator η_A such that $(v,(A_h-A)q_h) \le \eta_A \|\nabla v\|$ for all $v \in \mathring{H}^1(\Omega)$, we have

$$|\langle v, R_\Lambda\rangle| \le (\eta_{q_h} + \gamma^{-1}\eta_A)\,\|\nabla v\|_{L^2(\Omega)} + \Lambda\,\eta_{Nh}\left\|\nabla\Delta_N^{-1} v\right\|_{L^2(\Omega)} \qquad \textit{for all } v \in \mathring{H}^1(\Omega)\,. \tag{25}$$

Proof. For all $v \in \mathring{H}^1(\Omega)$ and $v_h \in \mathring{\mathcal{S}}$ we subtract (24) from the definition of the residual R_Λ to verify that

$$\begin{aligned}\langle v, R_\Lambda\rangle = {}& \gamma\,(\nabla(v_h - v), \nabla q_h) + \gamma^{-1}\,(v_h - v, f'(\widehat{\rho}_h)q_h + A_h\,q_h) - \Lambda\left(v_h - v, \Delta_{Nh}^{-1} q_h\right)\\ & - \Lambda\left(v, \Delta_{Nh}^{-1} q_h - \Delta_N^{-1} q_h\right) + \gamma^{-1}\,(v, (A_h - A)q_h)\ .\end{aligned}$$

An elementwise integration by parts and Hölder's inequality imply

$$\begin{aligned}|\langle v, R_\Lambda\rangle| \le {}& \sum_{K\in\mathcal{T}} \left\|h_{\mathcal{T}}^{-1}(v - v_h)\right\|_{L^2(K)} \left\|h_{\mathcal{T}}\left(\gamma\Delta q_h - \gamma^{-1}(f'(\widehat{\rho}_h)q_h + A_h q_h) + \Lambda\,\Delta_{Nh}^{-1} q_h\right)\right\|_{L^2(K)}\\ & + \sum_{E\in\mathcal{E}} \left\|h_{\mathcal{E}}^{-1/2}(v - v_h)\right\|_{L^2(E)} \left\|h_{\mathcal{E}}^{1/2}\gamma[\![\partial_{\vec{n}} q_h]\!]\right\|_{L^2(E)}\\ & + \Lambda\left|\left(v, \Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h\right)\right| + \gamma^{-1}\left|(v, (A_h - A)q_h)\right|\ .\end{aligned}$$

Choosing $v_h = \Pi_h v$ to be the Clément interpolant, with standard estimates and Lemma 4.1 we deduce (25). □

Let P_λ denote the L^2 projection onto the eigenspace related to the eigenvalue $-\lambda$, i.e. the space of all $q \in \mathring{H}^1(\Omega)$ satisfying (23). Choosing $v = q_h$ and $q = P_\lambda q_h$ in (23) leads to

$$0 = -\lambda\left(q_h, \Delta_N^{-1} P_\lambda q_h\right) + \gamma\,(\nabla q_h, \nabla P_\lambda q_h) + \gamma^{-1}\,(q_h, f'(\widehat{\rho}_h)P_\lambda q_h) + \gamma^{-1}\,(q_h, A\,P_\lambda q_h)\ .$$

We add this equation to the residual in Definition 4.2, where we choose $v = P_\lambda q_h$. Because Δ_N^{-1} is selfadjoint, i.e. $\left(P_\lambda q_h, \Delta_N^{-1} q_h\right) = -\left(\nabla\Delta_N^{-1} P_\lambda q_h, \nabla\Delta_N^{-1} q_h\right) = \left(\Delta_N^{-1} P_\lambda q_h, q_h\right)$, and A is assumed to be selfadjoint, we get a representation of the error in the eigenvalue approximation

$$\Lambda - \lambda = \frac{\langle P_\lambda q_h, R_\Lambda\rangle}{\left(P_\lambda q_h, \Delta_N^{-1} q_h\right)}\,, \tag{26}$$

provided that the denominator does not vanish. Thus the numerical approximation space has to be large enough to resolve the eigenvectors related to the principal eigenvalue, i.e. $P_\lambda\mathring{\mathcal{S}} \ne \{0\}$.

Theorem 4.4. *Let $-\lambda$ be the smallest number for which there exists a nontrivial q satisfying (23) and P_λ the L^2 projection onto the eigenspace related to $-\lambda$. Let $(\Lambda, q_h) \in (\mathbb{R}, \mathring{\mathcal{S}})$ solve (24) with $\left\|\nabla\Delta_{Nh}^{-1} q_h\right\|_{L^2(\Omega)} = 1$. Assume $\mathring{\mathcal{S}}$ is sufficiently large, such that*

$$\left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|_{L^2(\Omega)} \le \eta_{Nh} \le \frac{1}{4}\,, \tag{27}$$

and moreover

$$\left\|\nabla\Delta_N^{-1}(q_h - P_\lambda q_h)\right\|^2_{L^2(\Omega)} \le \frac{1}{4}\,. \tag{28}$$

Then, we have the following computable a posteriori error estimate for the eigenvalue

$$\lambda - \Lambda \le \eta_\Lambda := 8\gamma^{-1/2}(\eta_{q_h} + \eta_A)\left((\|f'(\widehat{\rho}_h)\|_\infty + \alpha)\,\|q_h\|^2 + 4\max(0, -\Lambda)\right)^{1/2} + 16\Lambda\eta_{Nh}\,. \tag{29}$$

Proof. For the denominator in (26), the assumed bound (28) implies

$$\begin{aligned} -2\left(P_\lambda q_h, \Delta_N^{-1} q_h\right) =& 2\left(\nabla\Delta_N^{-1} P_\lambda q_h, \nabla\Delta_N^{-1} q_h\right) \\ &= \left\|\nabla\Delta_N^{-1} P_\lambda q_h\right\|^2_{L^2(\Omega)} + \left\|\nabla\Delta_N^{-1} q_h\right\|^2_{L^2(\Omega)} - \left\|\nabla\Delta_N^{-1}(P_\lambda q_h - q_h)\right\|^2_{L^2(\Omega)} \\ &\geq 0 + \left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h) + \nabla\Delta_{Nh}^{-1} q_h\right\|^2_{L^2(\Omega)} - \frac{1}{4}, \\ &\geq \left(\left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|_{L^2(\Omega)} - \left\|\nabla\Delta_{Nh}^{-1} q_h\right\|_{L^2(\Omega)}\right)^2 - \frac{1}{4} \\ &= \left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|^2_{L^2(\Omega)} + \left\|\nabla\Delta_{Nh}^{-1} q_h\right\|^2_{L^2(\Omega)} \\ &\quad - 2\left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|_{L^2(\Omega)} \left\|\nabla\Delta_{Nh}^{-1} q_h\right\|_{L^2(\Omega)} - \frac{1}{4} \\ &\geq 0 + 1 - 2\cdot\frac{1}{4}\cdot 1 - \frac{1}{4} \quad = \quad \frac{1}{4}. \end{aligned}$$

Hence $\Lambda - \lambda \leq 8|\left\langle P_\lambda q_h, R_\Lambda\right\rangle|$. Now we apply Lemma 4.3, where we choose $v = P_\lambda q_h$ to conclude

$$\Lambda - \lambda \leq 8(\eta_{q_h} + \gamma^{-1}\eta_A)\left\|\nabla P_\lambda q_h\right\|_{L^2(\Omega)} + 8\Lambda\eta_{Nh}\left\|\nabla\Delta_N^{-1} P_\lambda q_h\right\|_{L^2(\Omega)}.$$

With (27), (28) and Lemma 4.1 we find that

$$\begin{aligned} \left\|\nabla\Delta_N^{-1} P_\lambda q_h\right\|_{L^2(\Omega)} &\leq \left\|\nabla\Delta_N^{-1}(P_\lambda q_h - q_h)\right\|_{L^2(\Omega)} + \left\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\right\|_{L^2(\Omega)} + \left\|\nabla\Delta_{Nh}^{-1} q_h\right\|_{L^2(\Omega)} \\ &\leq \frac{1}{2} + \eta_{Nh} + 1 \leq 2. \end{aligned} \tag{30}$$

To bound $\|\nabla P_\lambda q_h\|_{L^2(\Omega)}$ we choose $v = q = P_\lambda q_h$ in (23). This yields

$$\gamma\left\|\nabla P_\lambda q_h\right\|^2_{L^2(\Omega)} = -\lambda\left\|\nabla\Delta_N^{-1} P_\lambda q_h\right\|^2_{L^2(\Omega)} - \gamma^{-1}\left(P_\lambda q_h, f'(\widehat{\rho}_h) P_\lambda q_h + A P_\lambda q_h\right).$$

If $-\lambda \leq -\Lambda$ we use $\|P_\lambda q_h\|_{L^2(\Omega)} \leq \|q_h\|_{L^2(\Omega)}$ and (30) to verify

$$\gamma\left\|\nabla P_\lambda q_h\right\|^2_{L^2(\Omega)} \leq 4\max(0, -\Lambda) + \gamma^{-1}\left(\|f'(\widehat{\rho}_h)\|_\infty + \alpha\right)\|q_h\|^2$$

and deduce (29). Otherwise, if $\lambda \leq \Lambda$, nothing remains to be shown since the right-hand side of (29) is non-negative. □

The *saturation assumption* (28) in Theorem 4.4 is quite common to derive error estimates for eigenvalue approximation but it is not clear, how it can be verified in practice. To close this theoretical gap we present an explicit a priori estimate that only requires that the Laplace operator subject to homogeneous Neumann boundary conditions is H^2 regular on Ω, i.e. there is a constant $C_{H^2} > 0$ such that if $q, y \in \mathring{H}^1(\Omega)$ with $-\Delta y = q$ in Ω and $\partial_n y = 0$ on $\partial\Omega$, then $\|y\|_{H^2(\Omega)} \leq C_{H^2}\|q\|_{L^2(\Omega)}$. Instead of the difference $q_h - P_\lambda q$ in the a posteriori estimate, we now consider $q - \mathcal{I}_\mathcal{T} q$, where $\mathcal{I}_\mathcal{T}$ denotes the nodal interpolation operator. Then we have the interpolation estimate

$$\|q - \mathcal{I}_\mathcal{T} q\|_{L^2(\Omega)} + h\,\|\nabla(q - \mathcal{I}_\mathcal{T} q)\|_{L^2(\Omega)} \leq C_{\mathcal{I}_\mathcal{T}} h^2\left\|D^2 q\right\|_{L^2(\Omega)}. \tag{31}$$

Analogous to above, we need a suitable a priori estimate for $(A_h - A)q_h$. This can be obtained by standard methods, if A is the operator related to linear elasticity, cf. Lemma 5.3. From standard a priori estimates for the Laplace equation we get a constant $C_{Nh} > 0$ such that $\|\nabla(\Delta_N^{-1} q_h - \Delta_{Nh}^{-1} q_h)\|_{L^2(\Omega)} \leq C_{Nh} h\|q_h\|_{L^2(\Omega)}$ for all $q_h \in \mathring{\mathcal{S}}$. The optimal constant $C_{-1,1}$ such that $\|\nabla\Delta_N^{-1} v\|_{L^2(\Omega)} \leq C_{-1,1}^{-1}\|\nabla v\|_{L^2(\Omega)}$ for all $v \in \mathring{H}^1(\Omega)$ is needed to get an a priori estimate for the principal eigenvalue $-\lambda$. We note that $C_{-1,1}^{-1} \leq C_P^2$.

Theorem 4.5. *Assume that the Laplace operator subject to homogeneous Neumann boundary conditions is H^2 regular on Ω and suppose there is $C_{Ah} > 0$ such that $(q_h, (A_h - A)q_h) \leq C_{Ah} h \|\nabla q_h\|^2_{L^2(\Omega)}$ for all $q_h \in \mathring{\mathcal{S}}$. Set*

$$
\begin{aligned}
\varepsilon_0 &:= \gamma^2 + C_A + \max(C_P, C_P^2)\ \|f'(\widehat{\rho}_h)\|_{L^\infty(\Omega)}\ ,\\
\varepsilon_1 &:= \left(2\gamma^2\varepsilon_0 C^2_{-1,1} + 4(C_f + \alpha)^2\right)^{1/2}\ ,\\
\varepsilon_2 &:= \left(\varepsilon_0 C_{H^2}\left(\gamma^2 C^2_{-1,1} C_P\ + \varepsilon_1\right) C_{\mathcal{I}_\mathcal{T}}\, C_P/2\right)^{1/2}\ .
\end{aligned}
$$

Assume $\mathring{\mathcal{S}}$ is sufficiently large so that $2\gamma^{-2}\varepsilon_2\, h \leq 1/2$ as well, as $\gamma^{-1}(4\varepsilon_1^{1/2}\, C_P + \gamma) C_{Nh}\, h \leq C_P$ and define

$$
\begin{aligned}
\varepsilon_3 &:= 2\varepsilon_2 + C_{Nh}(4\gamma\varepsilon_1^{1/2} + \gamma^2/C_P)/2\\
\varepsilon_4 &:= \varepsilon_1\varepsilon_3 + \varepsilon_2(4\varepsilon_2 + \varepsilon_3/C_P)\,.
\end{aligned}
$$

Then, the error of the computed eigenvalue is bounded by

$$
\lambda - \Lambda \leq \gamma^{-7}\left[(2\gamma^2 + 6\varepsilon_0)(\varepsilon_1 + \varepsilon_4/(4\varepsilon_2))\,\varepsilon_4 + \gamma^2 C_{Ah}(\varepsilon_1 + \varepsilon_4/(4\varepsilon_2))^2\right] h\,.
$$

Proof. In a first step we derive a priori bounds for q and $|\lambda|$. From the definition of the principal eigenvalue $-\lambda$ in (9) and (A3) we get

$$
|\lambda| \leq \gamma^{-1}(\gamma^2 + C_P^2\ \|f'(\widehat{\rho}_h)\|_{L^\infty(\Omega)} + C_A) \inf_{v\in\mathring{H}^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2_{L^2(\Omega)}}{\left\|\nabla\Delta_N^{-1} v\right\|^2_{L^2(\Omega)}} \leq \gamma^{-1}\varepsilon_0 C^2_{-1,1}\,. \tag{32}
$$

Let (λ, q) satisfy (23) with $\left\|\nabla\Delta_N^{-1} q\right\|_{L^2(\Omega)} = 1$. We chose $v = q$ in (23) to infer with (A1), (A3) and (8) that

$$
\begin{aligned}
\gamma\|\nabla q\|^2_{L^2(\Omega)} &= -\lambda\left\|\nabla\Delta_N^{-1} q\right\|^2_{L^2(\Omega)} - \gamma^{-1}\,(q, f'(\widehat{\rho}_h) q)\ - \gamma^{-1}\,(q, Aq)\\
&\leq |\lambda| + \gamma^{-1}(C_f + \alpha)\,\|q\|^2_{L^2(\Omega)}\\
&\leq |\lambda| + 2\gamma^{-3}(C_f + \alpha)^2\left\|\nabla\Delta_N^{-1} q\right\|^2_{L^2(\Omega)} + \frac{\gamma}{2}\|\nabla q\|^2_{L^2(\Omega)}\ .
\end{aligned}
$$

From (32) we deduce the estimates

$$
\|\nabla q\|^2_{L^2(\Omega)} \leq 2\gamma^{-2}\varepsilon_0 C^2_{-1,1} + 4\gamma^{-4}(C_f + \alpha)^2\ = \gamma^{-4}\varepsilon_1^2\,, \tag{33}
$$

$$
\|q\|^2_{L^2(\Omega)} = -\left(\nabla\Delta_N^{-1} q, \nabla q\right) \leq \left\|\nabla\Delta_N^{-1} q\right\|_{L^2(\Omega)}\|\nabla q\|_{L^2(\Omega)} \leq \gamma^{-2}\varepsilon_1\,. \tag{34}
$$

We note $\left\|\Delta_N^{-1} q\right\|_{L^2(\Omega)} \leq C_P\left\|\nabla\Delta_N^{-1} q\right\|_{L^2(\Omega)} = C_P$ to conclude from the strong form $-\lambda\,\Delta_N^{-1} q = \gamma\Delta q - \gamma^{-1}(f'(\widehat{\rho}_h)\, q - A\, q)$ the assumed H^2 regularity that

$$
\begin{aligned}
\left\|D^2 q\right\|_{L^2(\Omega)} &\leq \gamma^{-1} C_{H^2}\left[|\lambda|\left\|\Delta_N^{-1} q\right\|_{L^2(\Omega)} + \gamma^{-1}\|f'(\widehat{\rho}_h) q + Aq\|_{L^2(\Omega)}\right]\\
&\leq \gamma^{-2} C_{H^2}\left[\gamma|\lambda|\, C_P + \left(C_P\ \|f'(\widehat{\rho}_h)\|_{L^\infty(\Omega)} + C_A\right)\|\nabla q\|_{L^2(\Omega)}\right]\\
&\leq \gamma^{-2} C_{H^2}\left(\varepsilon_0 C^2_{-1,1} C_P\ + \gamma^{-2}\varepsilon_0\varepsilon_1\right) \quad = \gamma^{-4}\, 2\varepsilon_2^2/(C_{\mathcal{I}_\mathcal{T}} C_P)\,.
\end{aligned}
$$

The second step consists in the construction of a discrete approximate eigenfunction. We define the meanvalue corrected nodal interpolant $\widetilde{\mathcal{I}}_\mathcal{T} q := \mathcal{I}_\mathcal{T} q - |\Omega|^{-1}\,(1, \mathcal{I}_\mathcal{T} q) \in \mathring{\mathcal{S}}$. Then, the triangle inequality and $q \in \mathring{H}^1(\Omega)$ lead to

$$
\|q - \widetilde{\mathcal{I}}_\mathcal{T} q\|_{L^2(\Omega)} \leq 2C_{\mathcal{I}_\mathcal{T}} h^2\left\|D^2 q\right\|_{L^2(\Omega)} \quad \leq 2h^2\ \gamma^{-4} 2\varepsilon_2^2/C_P\,.
$$

Since for any $v \in \mathring{H}^1(\Omega)$ we have $\left\|\nabla\Delta_N^{-1} v\right\|_{L^2(\Omega)} \leq C_P\,\|v\|_{L^2(\Omega)}$, the assumptions on the mesh width h yield

$$
\|\nabla\Delta_N^{-1}(q - \widetilde{\mathcal{I}}_\mathcal{T} q)\|_{L^2(\Omega)} \leq (2\gamma^{-2}\,\varepsilon_2\ \ h)^2 \leq 1/4\,. \tag{35}
$$

On the other hand, from the a priori estimate for Δ_N^{-1} we get

$$\begin{aligned}\|\nabla(\Delta_N^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q - \Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q)\|_{L^2(\Omega)} &\le C_{Nh}h\|\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}\\ &\le C_{Nh}h(\|q\|_{L^2(\Omega)} + \|q-\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)})\\ &\le C_{Nh}h(\gamma^{-1}\varepsilon_1^{1/2} + 1/(4C_P)) \ \le 1/4\,.\end{aligned}$$

Combining both estimates, from the triangle inequality we get $1/2 \le \|\nabla\Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)} \le 3/2$ so that we can define $\widetilde{q}_h := \widetilde{\mathcal{I}}_{\mathcal{T}}q/\|\nabla\Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}$ and deduce

$$\begin{aligned}\|\nabla(\widetilde{q}_h - q)\|_{L^2(\Omega)} &\le \frac{\left|1-\|\nabla\Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}\right|}{\|\nabla\Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}}\left\|\nabla\widetilde{\mathcal{I}}_{\mathcal{T}}q\right\|_{L^2(\Omega)} + \left\|\nabla(\widetilde{\mathcal{I}}_{\mathcal{T}}q - q)\right\|_{L^2(\Omega)}\\ &\le 2\left|\left\|\nabla\Delta_N^{-1}q\right\|_{L^2(\Omega)} - \|\nabla\Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}\right| \|\nabla\mathcal{I}_{\mathcal{T}}q\|_{L^2(\Omega)} + \|\nabla(\mathcal{I}_{\mathcal{T}}q-q)\|_{L^2(\Omega)}\\ &\le 2\left(\|\nabla\Delta_N^{-1}(q-\widetilde{\mathcal{I}}_{\mathcal{T}}q)\|_{L^2(\Omega)} + \|\nabla(\Delta_N^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q - \Delta_{Nh}^{-1}\widetilde{\mathcal{I}}_{\mathcal{T}}q\|_{L^2(\Omega)}\right)\|\nabla\mathcal{I}_{\mathcal{T}}q\|_{L^2(\Omega)}\\ &\quad + \|\nabla(\mathcal{I}_{\mathcal{T}}q-q)\|_{L^2(\Omega)}\\ &\le 2\left((2\gamma^{-2}\,\varepsilon_2\ \ h)^2 + C_{Nh}h(\gamma^{-1}\varepsilon_1^{1/2} + 1/(4C_P))\right)\|\nabla\mathcal{I}_{\mathcal{T}}q\|_{L^2(\Omega)}\\ &\quad + \|\nabla(\mathcal{I}_{\mathcal{T}}q-q)\|_{L^2(\Omega)}\ ,\\ &=: \gamma^{-2}\varepsilon_3 h\,\|\nabla\mathcal{I}_{\mathcal{T}}q\|_{L^2(\Omega)} + \|\nabla(\mathcal{I}_{\mathcal{T}}q-q)\|_{L^2(\Omega)}\ ,\end{aligned}$$

where we applied (35) and the assumption on the meshsize in order to reduce the polynomial dependence on γ^{-1}. From (33) and (31), we conclude

$$\begin{aligned}\|\nabla(\widetilde{q}_h - q)\|_{L^2(\Omega)} &\le \gamma^{-2}\varepsilon_3 h\,\|\nabla q\|_{L^2(\Omega)} + (1+\gamma^{-2}\varepsilon_3 h)\,\|\nabla(\mathcal{I}_{\mathcal{T}}q-q)\|_{L^2(\Omega)}\\ &\le \gamma^{-4}\varepsilon_1\varepsilon_3\,h + (1+\varepsilon_3/(4\varepsilon_2))4\gamma^{-4}(\varepsilon_2^2/C_P)h \quad =: \gamma^{-4}\varepsilon_4\,h\,.\end{aligned}$$

In the third step, we use the definitions of λ and Λ to estimate their difference. Setting $v_h = \widetilde{q}_h$ in (24) and using the minimality of $-\Lambda$ we get

$$-\Lambda \le \gamma\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2 + (\widetilde{q}_h, f'(\widehat{\rho}_h)\widetilde{q}_h) + (\widetilde{q}_h, A\widetilde{q}_h) + \gamma^{-1}\,(\widetilde{q}_h, (A_h - A)\widetilde{q}_h)\ . \tag{36}$$

Upon adding (23), where we chose $v = q$, we verify

$$\begin{aligned}\lambda - \Lambda \le&\gamma\left(\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2 - \|\nabla q\|_{L^2(\Omega)}^2\right) + \gamma^{-1}\Big((\widetilde{q}_h, f'(\widehat{\rho}_h)\widetilde{q}_h) - (q, f'(\widehat{\rho}_h)q) + (\widetilde{q}_h, A\widetilde{q}_h) - (q, Aq)\Big)\\ &+ \gamma^{-1}\,(\widetilde{q}_h, (A_h - A)\widetilde{q}_h)\ .\end{aligned}$$

In order to apply the binomial formula $a^2 - b^2 \le 2a(a-b)$, we define the shifted, positive definite operator $B := (f'(\widehat{\rho}_h) + \varepsilon_0 C_P^{-2})\,\mathrm{Id} + A$. This yields

$$\begin{aligned}\lambda - \Lambda \le&\gamma\left(\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2 - \|\nabla q\|_{L^2(\Omega)}^2\right) + \gamma^{-1}\Big((\widetilde{q}_h, B\widetilde{q}_h) - (q, Bq)\Big)\\ &- \gamma^{-1}\varepsilon_0 C_P^{-2}\left(\|\widetilde{q}_h\|_{L^2(\Omega)}^2 - \|q\|_{L^2(\Omega)}^2\right) + \gamma^{-1}\,(\widetilde{q}_h, (A_h - A)\widetilde{q}_h)\ .\end{aligned}$$

For the term containing $A_h - A$, we use the given a priori estimate from the assumptions to estimate

$$\begin{aligned}\lambda - \Lambda \le&2\gamma\,(\nabla\widetilde{q}_h, \nabla(\widetilde{q}_h - q)) + 2\gamma^{-1}\,(B\,\widetilde{q}_h, \widetilde{q}_h - q)\\ &+ 2\gamma^{-1}\varepsilon_0 C_P^{-2}\,(q, \widetilde{q}_h - q) + \gamma^{-1}C_{Ah}h\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2\\ \le&2\gamma\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}\,\|\nabla(\widetilde{q}_h - q)\|_{L^2(\Omega)} + 2\gamma^{-1}2\varepsilon_0\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}\,\|\nabla(\widetilde{q}_h - q)\|_{L^2(\Omega)}\\ &+ 2\gamma^{-1}\varepsilon_0 C_P^{-2}\,\|q\|_{L^2(\Omega)}\,\|\widetilde{q}_h - q\|_{L^2(\Omega)} + \gamma^{-1}C_{Ah}h\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2\\ \le&2\Big[\gamma\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)} + 2\gamma^{-1}\varepsilon_0\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)} + \gamma^{-1}\varepsilon_0\,\|\nabla q\|_{L^2(\Omega)}\Big]\,\gamma^{-4}\varepsilon_4\,h\\ &+ \gamma^{-1}C_{Ah}h\,\|\nabla\widetilde{q}_h\|_{L^2(\Omega)}^2\ .\end{aligned}$$

We finally note $\|\nabla\widetilde{q}_h\|_{L^2(\Omega)} \le \gamma^{-2}(\varepsilon_1 + \varepsilon_4/(4\varepsilon_2))$ to verify the desired estimate. □

5 Application to Homogeneous Elasticity

The last missing parts to gain robust error control are the residual estimators. These depend on the concrete application with a particular linear operator A and on the implemented numerical method. In this section we present a practical method for a semi-implicit treatment of the general Cahn-Larché system and derive computable residual estimators in the case of a homogeneous elasticity tensor.

5.1 Homogeneous Elasticity

Let the elasticity tensor $\mathcal{C} \in \mathbb{R}^{d\times d\times d\times d}$ be a symmetric positive definite fourth order tensor, i.e.

- $\mathcal{C}_{ijmn} = \mathcal{C}_{ijnm} = \mathcal{C}_{jimn}$ and $\mathcal{C}_{ijmn} = \mathcal{C}_{mnij}$ for all $1 \le i,j,m,n \le d$,
- there is $c^* > 0$, such that $\mathcal{A} : \mathcal{C}\mathcal{A} \ge c^* |\mathcal{A}|^2$ for all symmetric matrices $\mathcal{A} \in \mathbb{R}^{d\times d}$.

For symmetric matrices $\mathcal{A}, \mathcal{B}$ we define $\mathcal{A} : \mathcal{B} := \operatorname{trace}\left(\mathcal{A}^T\mathcal{B}\right) = \sum_{i,j} \mathcal{A}_{ij}\mathcal{B}_{ij}$ and the scalar product $(\mathcal{A},\mathcal{B})_{\mathcal{C}} := \int_\Omega \mathcal{A} : \mathcal{C}\mathcal{B}\,\mathrm{d}x$. The set of all infinitesimal, linearized rigid body motions is given by

$$\mathrm{RM}(\Omega) = \begin{cases} \{(x,y) \mapsto (a,b) + c(y,-x) : a,b,c \in \mathbb{R},\ (x,y) \in \Omega \subset \mathbb{R}^2\} & \text{for } d = 2\,, \\ \{x \mapsto a + c \times x : a,b \in \mathbb{R}^3,\ x \in \Omega \subset \mathbb{R}^3\} & \text{for } d = 3\,. \end{cases}$$

By $H^1_{\mathrm{RM}}(\Omega)$ we denote the subspace of $\left(H^1(\Omega)\right)^d$ where all linearized rigid body motions have been removed and define the solution space of the Cahn-Larché system by

$$X_{\mathrm{CL}} := X_{\mathrm{CH}} \times L^\infty([0,T], H^1_{\mathrm{RM}}(\Omega))\,.$$

In the weak form we seek the solution of the following problem

$$(\mathbf{CL}) \begin{cases} \text{Given } \rho(0,x) = \rho_0(x) \in H^1(\Omega),\ \text{find } (\rho,w,\vec{u}) \in X_{\mathrm{CL}} \text{ such that for almost all } t \in (0,T) \\ \left(\mathcal{E}(\vec{\xi}), \mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right)_{\mathcal{C}} = 0 & \text{for all } \vec{\xi} \in H^1_{\mathrm{RM}}(\Omega)\,, \\ \langle \varphi, \partial_t \rho\rangle + (\nabla\varphi, \nabla w) = 0 & \text{for all } \varphi \in H^1(\Omega)\,, \\ (\psi, w) - \gamma\,(\nabla\psi, \nabla\rho) = \gamma^{-1}\,(\psi, f(\rho) + W(\rho, \mathcal{E}(\vec{u}))) & \text{for all } \psi \in H^1(\Omega)\,. \end{cases}$$

Following [15], the elastic energy can be modeled by

$$\mathcal{W}(\rho, \mathcal{E}(\vec{u})) := \frac{1}{2}\left(\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right) : \mathcal{C}\left(\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right)\,.$$

If the elasticity tensor $\mathcal{C}$ is homogeneous, the first equation of (CL) defines the linear solution operator $\mathcal{D}^{-1} : \rho \mapsto \vec{u}$ and the contribution of the elastic energy to (CL) is

$$W(\rho, \mathcal{E}(\vec{u})) = -\kappa\mathbb{I} : \mathcal{C}\left(\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right)\,. \tag{37}$$

In the next lemma, we show that the mapping $\rho \mapsto A\rho = W(\rho, \mathcal{E}(\vec{u}))$ satisfies (A3).

Lemma 5.1. *There is a constant $C_{\mathcal{C},K}$ such that for given $\rho \in L^2(\Omega)$ and $\vec{u}$ as in (CL) we have*

$$\|\nabla\vec{u}\|_{L^2(\Omega)} \le \kappa\, C_{\mathcal{C},K}\, \|\rho\|_{L^2(\Omega)}\,. \tag{38}$$

Moreover, the linear operator $A : \rho \mapsto W(\rho, \mathcal{E}(\vec{u})) = -\kappa\mathbb{I} : \mathcal{C}\left(\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right)$ is selfadjoint and there are constants $\alpha, C_A \ge 0$ such that assumption (A3) is satisfied, i.e.

$$\begin{aligned} -(\rho, A\rho) &\le \alpha\,\|\rho\|^2_{L^2(\Omega)} && \textit{for all } \rho \in L^2(\Omega)\,, \\ (\psi, A\rho) &\le C_A\,\|\nabla\psi\|_{L^2(\Omega)}\,\|\nabla\rho\|_{L^2(\Omega)} && \textit{for all } \rho \in \mathring{H}^1(\Omega)\,. \end{aligned}$$

Proof. Since we excluded rigid body motions, we can apply Korn's inequality. On the other hand, $\mathcal{C}$ is positive definite, together this yields

$$C_K \, \|\nabla \vec{u}\|^2_{L^2(\Omega)} \le (\mathcal{E}(\vec{u}), \mathcal{E}(\vec{u})) \le \frac{1}{c^*} \, (\mathcal{E}(\vec{u}), \mathcal{E}(\vec{u}))_{\mathcal{C}} \; . \tag{39}$$

By choosing $\vec{\xi} = \vec{u}$ in (CL) and employing Hölder's inequality we verify

$$\begin{aligned}\|\nabla \vec{u}\|^2_{L^2(\Omega)} &\le \frac{1}{c^* \, C_K} \left(\bar{\mathcal{E}}(\rho), \mathcal{E}(\vec{u})\right)_{\mathcal{C}} = \frac{\kappa}{c^* \, C_K} \int_\Omega \rho \; \mathcal{E}(\vec{u}) : \mathcal{C}\mathbb{I} \, dx \\ &\le \frac{\kappa}{c^* \, C_K} \, \|\rho\|_{L^2(\Omega)} \, \|\mathcal{E}(\vec{u}) : \mathcal{C}\mathbb{I}\|_{L^2(\Omega)} \le \kappa \, C_{\mathcal{C},K} \, \|\rho\|_{L^2(\Omega)} \, \|\nabla \vec{u}\|_{L^2(\Omega)} \; ,\end{aligned}$$

with some constant $C_{\mathcal{C},K} > 0$. The symmetry of $\mathcal{C}$ implies that A is selfadjoint and

$$\begin{aligned}(\rho, A\rho) &= -\int_\Omega \kappa \mathbb{I} \rho : \mathcal{C} \left(\mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right) dx = -\left(\bar{\mathcal{E}}(\rho), \mathcal{E}(\vec{u}) - \bar{\mathcal{E}}(\rho)\right)_{\mathcal{C}} \\ &= -\left(\mathcal{E}(\vec{u}), \mathcal{E}(\vec{u})\right)_{\mathcal{C}} + \left(\bar{\mathcal{E}}(\rho), \bar{\mathcal{E}}(\rho)\right)_{\mathcal{C}} \ge -c^* \, C_K \, \|\nabla \vec{u}\|^2_{L^2(\Omega)} + \kappa^2 c^* \, \|\rho\|^2_{L^2(\Omega)} \; .\end{aligned}$$

Upon setting $\alpha = \max(0, \kappa^2 \, (C_K \, C^2_{\mathcal{C},K} - |\Omega|)) \, c^*$ we get the lower bound for A. For the upper bound, we set $\vec{\xi} = \mathcal{D}^{-1}\psi$ and $\vec{v} = \mathcal{D}^{-1}\rho$. An application of Hölder's inequality, (38) and (39) yield

$$\begin{aligned}(\psi, A\rho) &= -\left(\bar{\mathcal{E}}(\psi), \mathcal{E}(\vec{v}) - \bar{\mathcal{E}}(\rho)\right)_{\mathcal{C}} = -\left(\mathcal{E}(\vec{\xi}), \mathcal{E}(\vec{v})\right)_{\mathcal{C}} + \left(\bar{\mathcal{E}}(\psi), \bar{\mathcal{E}}(\rho)\right)_{\mathcal{C}} \\ &\le \left(\mathcal{E}(\vec{\xi}), \mathcal{E}(\vec{\xi})\right)^{1/2}_{\mathcal{C}} \left(\mathcal{E}(\vec{v}), \mathcal{E}(\vec{v})\right)^{1/2}_{\mathcal{C}} + \kappa^2 \mathbb{I} : \mathcal{C}\mathbb{I} \, \|\psi\|_{L2} \, \|\rho\|_{L^2(\Omega)} \\ &\le C_K^2 \|\nabla \vec{\xi}\|_{L^2(\Omega)} \|\nabla \vec{\xi}\|_{L^2(\Omega)} + \kappa^2 \mathbb{I} : \mathcal{C}\mathbb{I} C_P^2 \, \|\nabla \psi\|_{L2} \, \|\nabla \rho\|_{L^2(\Omega)} \\ &\le (C_K^2 \, \kappa^2 \, C^2_{\mathcal{C},K} + \kappa^2 \mathbb{I} : \mathcal{C}\mathbb{I} C_P^2) \, \|\nabla \psi\|_{L2} \, \|\nabla \rho\|_{L^2(\Omega)} \; .\end{aligned}$$

□

5.2 Numerical Scheme and Residual Estimates

We define $\mathcal{S}_{\mathrm{RM}} := \mathcal{S}^d \cap H^1_{\mathrm{RM}}(\Omega)$ and propose the following decoupled semi-implicit numerical method to approximate (CL):

$$(\mathbf{CL_h}) \begin{cases} \text{Given the approximations } \rho_h^{(j-1)} \text{ at time } t_{j-1}, \text{ first compute } \vec{u}_h^{(j)} \in \mathcal{S}^{(j)}_{\mathrm{RM}} \text{ such that} \\ \qquad 0 = \left(\mathcal{E}(\vec{\xi}_h), \mathcal{E}(\vec{u}_h^{(j)}) - \bar{\mathcal{E}}(\mathcal{I}^{(j)} \rho_h^{(j-1)})\right)_{\mathcal{C}} \qquad \text{for all } \vec{\xi}_h \in \mathcal{S}^{(j)}_{\mathrm{RM}} \,, \\ \text{then compute } (\rho_h^{(j)}, w_h^{(j)}) \in \mathcal{S}^{(j)} \times \mathcal{S}^{(j)} \text{ such that} \\ \left(\varphi_h, \rho_h^{(j)}\right) + \tau_j \left(\nabla \varphi_h, \nabla w_h^{(j)}\right) = \left(\varphi_h, \mathcal{I}^{(j)} \rho_h^{(j-1)}\right) \qquad \text{for all } \varphi_h \in \mathcal{S}^{(j)} \,, \\ \left(\psi_h, w_h^{(j)}\right) - \gamma \left(\nabla \psi_h, \nabla \rho_h^{(j)}\right) - \gamma^{-1} \left(\psi_h, f'(\mathcal{I}^{(j)} \rho_h^{(j-1)}) \rho_h^{(j)}\right) \\ \qquad = \gamma^{-1} \left(\psi_h, f(\mathcal{I}^{(j)} \rho_h^{(j-1)}) - f'(\mathcal{I}^{(j)} \rho_h^{(j-1)}) \rho_h^{(j-1)}\right) \\ \qquad + \gamma^{-1} \left(\psi_h, W(\mathcal{I}^{(j)} \rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)}))\right) \qquad \text{for all } \psi_h \in \mathcal{S}^{(j)} \,. \end{cases}$$

Definition 5.2. Given $\rho_h \in L^2(\Omega)$ and $\vec{u}_h$ the finite element solution of $0 = \left(\mathcal{E}(\vec{\xi}_h), \mathcal{E}(\vec{u}_h) - \bar{\mathcal{E}}(\rho_h)\right)_{\mathcal{C}}$ for all $\vec{\xi}_h \in \mathcal{S}_{\mathrm{RM}}$ the *residual* R_3 is defined as

$$\langle \vec{\xi}, R_3 \rangle := \left(\mathcal{E}(\vec{\xi}), \mathcal{E}(\vec{u}_h) - \bar{\mathcal{E}}(\rho_h)\right)_{\mathcal{C}} \qquad \text{for all } \vec{\xi} \in H^1_{\mathrm{RM}}(\Omega) \,. \tag{40}$$

Lemma 5.3. *Suppose $\mathcal{C}$ is homogeneous and $W(\rho,\mathcal{E}(\vec{u}))$ given by (37). Let $A:\rho\mapsto W(\rho,\mathcal{E}(\vec{u}))$ with $\vec{u}$ defined by the first identity in (CL). Similarly, let $A_h:\rho_h\mapsto W(\rho_h,\mathcal{E}(\vec{u}_h))$ with $\vec{u}_h$ as in Definition 5.2. Set*

$$\widetilde{\eta}_A := \left\| h_{\mathcal{T}}\Big(\operatorname{div}_{\mathcal{T}}\left(\mathcal{C}\left[\mathcal{E}(\vec{u}_h)-\bar{\mathcal{E}}(\rho_h)\right]\right)\Big)\right\|_{L^2(\Omega)} + \left\| h_{\mathcal{E}}^{1/2}\left[\!\left[\vec{n}\cdot\left(\mathcal{C}\mathcal{E}(\vec{u}_h)-\bar{\mathcal{E}}(\rho_h)\right)\right]\!\right]\right\|_{L^2(\cup\mathcal{E})} .$$

Then, with $\eta_A := \kappa\, C_P C_{\mathcal{C},K} C_{Cl}\,\widetilde{\eta}_A$, we have

$$\begin{aligned} \langle\vec{\xi},R_3\rangle &\le \widetilde{\eta}_A\, C_{Cl}\|\nabla\vec{\xi}\|_{L^2(\Omega)} && \textit{for all } \vec{\xi}\in H^1_{RM}(\Omega)\,,\\ (\varphi,(A_h-A)\rho_h) &\le \eta_A\ \|\nabla\varphi\|_{L^2(\Omega)} && \textit{for all } \varphi\in \mathring{H}^1(\Omega)\,. \end{aligned} \tag{41}$$

Under the assumption of H^2 regularity of the elasticity equations in the sense that $\|\vec{u}\|_{H^2(\Omega)}\le C\,\|\nabla\rho_h\|_{L^2(\Omega)}$, there is a constant $C_{Ah}>0$ such that we have the a priori estimate

$$|\,(\rho_h,(A_h-A)\rho_h)\,| \le C_{Ah}\,h\,\|\nabla\rho_h\|^2_{L^2(\Omega)}\ .$$

Proof. Let $\vec{\xi}\in H^1_{\mathrm{RM}}(\Omega)$. By Galerkin orthogonality we can insert the Clément interpolant of $\vec{\xi}$ in (40). Using elementwise integration by parts and applying standard estimates we get

$$\langle\vec{\xi},R_3\rangle \le \widetilde{\eta}_A\, C_{Cl}\|\nabla\vec{\xi}\|_{L^2(\Omega)}\,.$$

Define $\vec{v}:=\mathcal{D}^{-1}\rho_h$, then $A\,\rho_h = -\kappa\mathbb{I}:\mathcal{C}\left(\mathcal{E}(\vec{v})-\bar{\mathcal{E}}(\rho_h)\right)$ and for $\varphi\in\mathring{H}^1(\Omega)$ set $\vec{\xi}:=\mathcal{D}^{-1}\varphi$. Since $\vec{u}_h-\vec{v}\in H^1_{\mathrm{RM}}(\Omega)$ is an admissible test function, we verify

$$\begin{aligned}(\varphi,(A_h-A)\rho_h) &= \left(\bar{\mathcal{E}}(\varphi),\mathcal{E}(\vec{u}_h)-\mathcal{E}(\vec{v})\right)_{\mathcal{C}}\\ &= \Big(\mathcal{E}(\vec{\xi}),\mathcal{E}(\vec{u}_h)-\mathcal{E}(\vec{v})\Big)_{\mathcal{C}} = \Big(\mathcal{E}(\vec{\xi}),\mathcal{E}(\vec{u}_h)-\bar{\mathcal{E}}(\rho_h)\Big)_{\mathcal{C}} = \Big\langle\vec{\xi},R_3\Big\rangle\ .\end{aligned}$$

With Lemma 5.1 and Poincaré's inequality we infer (41). For the a priori estimate, we choose $\varphi=\rho_h$ and apply Hölder's inequality to deduce

$$\begin{aligned}|\,(\rho_h,(A_h-A)\rho_h)\,| = |\,(\mathcal{E}(\vec{v}),\mathcal{E}(\vec{u}_h)-\mathcal{E}(\vec{v}))_{\mathcal{C}}\,| &\le (\mathcal{E}(\vec{v}),\mathcal{E}(\vec{v}))^{1/2}_{\mathcal{C}}\ (\mathcal{E}(\vec{u}_h-\vec{v}),\mathcal{E}(\vec{u}_h-\vec{v}))^{1/2}_{\mathcal{C}}\\ &\le c^*\,C_K\ \|\nabla\vec{v}\|\ C\,h\ \left\|D^2\vec{v}\right\|_{L^2(\Omega)}\ ,\end{aligned}$$

due to (39) and standard a priori estimates for linear elasticity with a constant $C>0$. Then, we finish the proof by using (38) and the H^2 regularity of $\vec{v}$. □

Lemma 5.4. *Let $(\rho_h^{(j)},w_h^{(j)},u_h^{(j)})_{j=0,\cdots N}$ be the solution of* (CL$_\mathrm{h}$) *and let (ρ_h,w_h,u_h) denote the piecewise affine in time interpolation. Set $r^{(j)}:=\max(\|\rho_h^{(j-1)}\|_{L^\infty(\Omega)},\|\rho_h^{(j)}\|_{L^\infty(\Omega)})$ and $I^{(j)}:=[-r^{(j)},r^{(j)}]$. Let $\eta_A^{(j)}$ be as in Lemma 5.3. Define the residual estimators*

$\eta_1^{(j)}:=C_{Cl}\,\eta_{1h}^{(j)}+\eta_{1t}^{(j)}+\eta_{1c}^{(j)}$, where

$$\begin{aligned}\eta_{1h}^{(j)} &:= \left\|h_{\mathcal{T}^{(j)}}\left(\tau_j^{-1}\left(\rho_h^{(j)}-\mathcal{I}^{(j)}\rho_h^{(j-1)}\right)-\Delta w_h^{(j)}\right)\right\|_{L^2(\Omega)} + \left\|h_{\mathcal{E}^{(j)}}^{1/2}\left[\!\left[\partial_{\vec{n}}w_h^{(j)}\right]\!\right]\right\|_{L^2(\cup\mathcal{E}^{(j)})}\ ,\\ \eta_{1t}^{(j)} &:= C_P\left\|\nabla w_h^{(j)}-\nabla w_h^{(j-1)}\right\|_{L^2(\Omega)}\ ,\\ \eta_{1c}^{(j)} &:= \tau_j^{-1}C_P\left\|\mathcal{I}^{(j)}\rho_h^{(j-1)}-\rho_h^{(j-1)}\right\|_{L^2(\Omega)}\ ,\end{aligned}$$

$\eta_{21}^{(j)}:=C_{Cl}\,\eta_{21h}^{(j)}+\eta_{21t}^{(j)}+(\eta_A^{(j-1)}+\eta_A^{(j)})$, where

$$\begin{aligned}\eta_{21h}^{(j)} := \Bigg\|h_{\mathcal{T}^{(j)}}\Big(w_h^{(j)}+\gamma\Delta_{\mathcal{T}^{(j)}}\rho_h^{(j)}-\gamma^{-1}\Big[f(\mathcal{I}^{(j)}\rho_h^{(j-1)})+W(\mathcal{I}^{(j)}\rho_h^{(j-1)},\mathcal{E}(\vec{u}_h^{(j)}))\\ +f'(\mathcal{I}^{(j)}\rho_h^{(j-1)})(\rho_h^{(j)}-\mathcal{I}^{(j)}\rho_h^{(j-1)})\Big]\Big)\Bigg\|_{L^2(\Omega)} + \gamma\left\|h_{\mathcal{E}^{(j)}}^{1/2}\left[\!\left[\partial_{\vec{n}}\rho_h^{(j)}\right]\!\right]\right\|_{L^2(\cup\mathcal{E}^{(j)})}\ ,\\ \eta_{21t}^{(j)} := \gamma\left\|\nabla(\rho_h^{(j)}-\rho_h^{(j-1)})\right\|_{L^2(\Omega)}\ ,\end{aligned}$$

$$
\begin{aligned}
\eta_{22}^{(j)} &:= \eta_{2t}^{(j)} + \eta_{2c}^{(j)} + \eta_{2\ell}^{(j)}\,,\\
\eta_{22t}^{(j)} &:= \left\| w_h^{(j)} - w_h^{(j-1)} \right\|_{L^2(\Omega)} + \gamma^{-1} \|f'\|_{L^\infty(I^{(j)})} \|\rho_h^{(j)} - \rho_h^{(j-1)}\|_{L^2(\Omega)}\\
&\quad + \gamma^{-1} \left\| W(\rho_h^{(j)}, \mathcal{E}(\vec{u}_h^{(j)})) - W(\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) \right\|_{L^2(\Omega)}\,,\\
\eta_{2c}^{(j)} &:= \gamma^{-1} \left\| W(\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) - W(\mathcal{I}^{(j)}\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) \right\|_{L^2(\Omega)}\\
\eta_{2\ell}^{(j)} &:= \gamma^{-1} \left\| f(\rho_h^{(j)}) - f(\mathcal{I}^{(j)}\rho_h^{(j-1)}) - f'(\mathcal{I}^{(j)}\rho_h^{(j-1)}) \left[\rho_h^{(j)} - \rho_h^{(j-1)}\right] \right\|_{L^2(\Omega)}\,.
\end{aligned}
$$

Then, for almost all $s \in (t_{j-1}, t_j)$, $j = 1, \cdots, N$, we have

$$\langle \varphi, R_1(s) \rangle \le \eta_1^{(j)} \|\nabla\varphi\|_{L^2(\Omega)} \qquad \text{for all } \varphi \in \mathring{H}^1(\Omega)\,, \tag{42a}$$

$$\langle \psi, R_2(s) \rangle \le \eta_{21}^{(j)} \|\nabla\psi\|_{L^2(\Omega)} + \eta_{22}^{(j)} \|\psi\|_{L^2(\Omega)} \qquad \text{for all } \psi \in \mathring{H}^1(\Omega)\,, \tag{42b}$$

Proof. We add and subtract terms to the residuals defined in Definition 2.2, such that we split the residuals into $R_1(s) = R_{1h}^{(j)} + R_{1t}(s) + R_{1c}^{(j)}$ and $R_2(s) = R_{2h}^{(j)} + R_{2t}(s) + R_{2c}^{(j)} + R_{2\ell}^{(j)} + (A - A_h)\rho_h$, where the subscripts c, ℓ, h and t refer to coarsening-, linearization-, space discretization-, and time discretization residuals, respectively. Since ρ_h and is affine in (t_{j-1}, t_j), with Lemma 5.3 we can directly estimate $(\psi, (A - A_h)\rho_h(s)) \le (\eta_A^{(j)} + \eta_A^{(j-1)}) \|\nabla\psi\|_{L^2(\Omega)}$. The space discretization residuals are given by the discrete operator applied to test functions in the whole space $\mathring{H}^1(\Omega)$

$$\left\langle \varphi, R_{1h}^{(j)} \right\rangle := \tau_j^{-1} \left(\varphi, \rho_h^{(j)} - \mathcal{I}^{(j)}\rho_h^{(j-1)} \right) + \left(\nabla\varphi, \nabla w_h^{(j)} \right)\,, \tag{43a}$$

$$
\begin{aligned}
\left\langle \psi, R_{2h}^{(j)} \right\rangle :=& \gamma \left(\nabla\psi, \nabla\rho_h^{(j)} \right) + \gamma^{-1} \left(\psi, f'(\mathcal{I}^{(j)}\rho_h^{(j-1)})(\rho_h^{(j)} - \mathcal{I}^{(j)}\rho_h^{(j-1)}) \right) - \left(\psi, w_h^{(j)} \right)\\
&+ \gamma^{-1} \left(\psi, f(\mathcal{I}^{(j)}\rho_h^{(j-1)}) + W(\mathcal{I}^{(j)}\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) \right)\,.
\end{aligned} \tag{43b}
$$

The linearization residual is

$$\left\langle \psi, R_{2\ell}^{(j)} \right\rangle := \gamma^{-1} \left(\psi_h, f(\rho_h^{(j)}) - f(\mathcal{I}^{(j)}\rho_h^{(j-1)}) - f'(\mathcal{I}^{(j)}\rho_h^{(j-1)}) \left[\rho_h^{(j)} - \mathcal{I}^{(j)}\rho_h^{(j-1)} \right] \right) \tag{44}$$

and the coarsening residuals contain the remaining explicit terms in the scheme, i.e.

$$\left\langle \varphi, R_{1c}^{(j)} \right\rangle := \tau_j^{-1} \left(\varphi, \mathcal{I}^{(j)}\rho_h^{(j-1)} - \rho_h^{(j-1)} \right)\,, \tag{45a}$$

$$\left\langle \varphi, R_{2c}^{(j)} \right\rangle := \gamma^{-1} \left(\varphi, W(\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) - W(\mathcal{I}^{(j)}\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) \right)\,. \tag{45b}$$

Finally, the time discretization residuals are given by

$$\langle \varphi, R_{1t}(s) \rangle := \left(\nabla\varphi, \nabla w_h(s) - \nabla w_h^{(j)} \right)\,, \tag{46a}$$

$$
\begin{aligned}
\langle \psi, R_{2t}(s) \rangle :=& \gamma \left(\nabla\psi, \nabla\rho_h(s) - \nabla\rho_h^{(j)} \right) - \left(\psi, w_h(s) - w_h^{(j)} \right)\\
&+ \gamma^{-1} \left(\psi, f(\rho_h(s)) - f(\rho_h^{(j)}) + W(\rho_h(s), \mathcal{E}(\vec{u}_h(s))) - W(\rho_h^{(j-1)}, \mathcal{E}(\vec{u}_h^{(j)})) \right)\,.
\end{aligned} \tag{46b}
$$

By Galerkin orthogonality we can insert the Clément interpolant $\Pi_h\varphi$ into the space discretization residual $R_{1h}^{(j)}$. Then, with elementwise integration by parts and standard estimates we conclude

$$
\begin{aligned}
\left\langle \varphi, R_{1h}^{(j)} \right\rangle &= \sum_{K \in \mathcal{T}^{(j)}} \left(\varphi - \Pi_h\varphi, \tau_j^{-1} \left(\rho_h^{(j)} - \mathcal{I}^{(j)}\rho_h^{(j-1)} \right) - \Delta_{\mathcal{T}^{(j)}} w_h \right) + \sum_{E \in \mathcal{E}^{(j)}} (\varphi - \Pi_h\varphi, [\![\partial_{\vec{n}} w_h]\!])\\
&\le C_{Cl}\, \eta_{1h} \|\nabla\varphi\|_{L^2(\Omega)}\,.
\end{aligned}
$$

Analogously, we infer $\langle \psi, R_{2h}^{(j)} \rangle \le C_{Cl}\, \eta_{21h} \|\psi\|_{L^2(\Omega)}$. Since ρ_h and w_h are affine in (t_{j-1}, t_j), by Hölders's and Poincaré's inequality we conclude

$$\langle \varphi, R_{1c} \rangle \le \tau_j^{-1} \|\mathcal{I}^{(j)}\rho_h^{(j-1)} - \rho_h^{(j-1)}\|_{L^2(\Omega)} \|\varphi\|_{L^2(\Omega)} \le \eta_{1c} \|\nabla\varphi\|_{L^2(\Omega)}$$

in analogous way $\langle\varphi, R_{1t}^{(j)}\rangle \leq \eta_{1t}^{(j)} \|\nabla\varphi\|_{L^2(\Omega)}$. Further application of Hölder's inequality proves $\langle\psi, R_{2\ell}^{(j)}\rangle \leq \eta_{2\ell}^{(j)} \|\psi\|_{L^2(\Omega)}$ and $\langle\psi, R_{2c}^{(j)}\rangle \leq \eta_{2c}^{(j)} \|\psi\|_{L^2(\Omega)}$. The first term of the time discretization residual $R_{2t}(s)$ is estimated with η_{21t}. W is linear with respect to $\mathcal{E}(\vec{u})$ and for each $x \in \Omega$ there is some r_x between $\rho_h(s,x)$ and $\rho_h^{(j)}(x)$ such that

$$f(\rho_h(s,x)) - f(\rho_h^{(j)}(x)) = f'(r_x)\left(\rho_h(s,x) - \rho_h^{(j)}(x)\right) \leq \|f'\|_{L^\infty(I^{(j)})}|\rho_h^{(j)}(x) - \rho_h^{(j-1)}(x)|\,.$$

Then, by Hölder's inequality we deduce $\langle\psi, R_{2t}^{(j)}\rangle \leq \eta_{21t}^{(j)} \|\nabla\psi\|_{L^2(\Omega)} + \eta_{22t}^{(j)} \|\psi\|_{L^2(\Omega)}$. □

6 Numerical Experiments

In this section we illustrate the theoretical results of the previous sections and discuss analytical properties of the given equations. The numerical experiments also show that the given error indicators, the grid adaption and coarsening strategy enables an efficient and accurate solution of the Cahn-Larché system. We used the numerical method ($\mathrm{CL_h}$) to approximate the time evolution. The discrete eigenvalue problem in the jth time step reads as follows:

$$(\mathbf{EV_h})\begin{cases} \text{Given } \rho_h^{(j)}, \text{ find } (q_h, z_h, \vec{v}_h, \Lambda) \in \mathcal{S}^{(j)} \times \mathcal{S}^{(j)} \times \mathcal{S}_{\mathrm{RM}}^{(j)} \times \mathbb{R} \text{ such that} \\ \left(\mathcal{E}(\vec{\xi}_h), \mathcal{E}(\vec{v}_h) - \bar{\mathcal{E}}(q_h)\right)_{\mathcal{C}} = 0 \qquad \text{for all } \vec{\xi}_h \in \mathcal{S}_{\mathrm{RM}}^{(j)}\,, \\ \gamma\,(\varphi_h, q_h) - \gamma\,(\nabla\varphi_h, \nabla z_h) = 0 \qquad \text{for all } \varphi_h \in \mathring{\mathcal{S}}^{(j)}\,, \\ \gamma\,(\nabla\psi_h, \nabla q_h) + \gamma^{-1}\left(\psi_h, f'(\rho_h^{(j)})q_h + W(q_h, \mathcal{E}(\vec{v}_h))\right) = -\Lambda\,(\psi_h, z_h) \qquad \text{for all } \psi_h \in \mathring{\mathcal{S}}^{(j)}\,. \end{cases}$$

We solve this problem by a shifted inverse vector iteration. Therefore, we introduce a term $\varepsilon_0\,(\psi_h, z_h)$ to each side of the last equation of ($\mathrm{EV_h}$). We note that the eigenvalue problem can not be decoupled into an elasticity part and a Cahn-Hilliard part, so the size of the linear system to solve is twice as large compared to each subproblem in ($\mathrm{CL_h}$). Due to the constraints related to the spaces $\mathring{\mathcal{S}}^{(j)}$ and $\mathcal{S}_{\mathrm{RM}}^{(j)}$ this matrix has a large bandwidth, thus it is not well suited for direct solvers.

6.1 Detection of Topological Changes

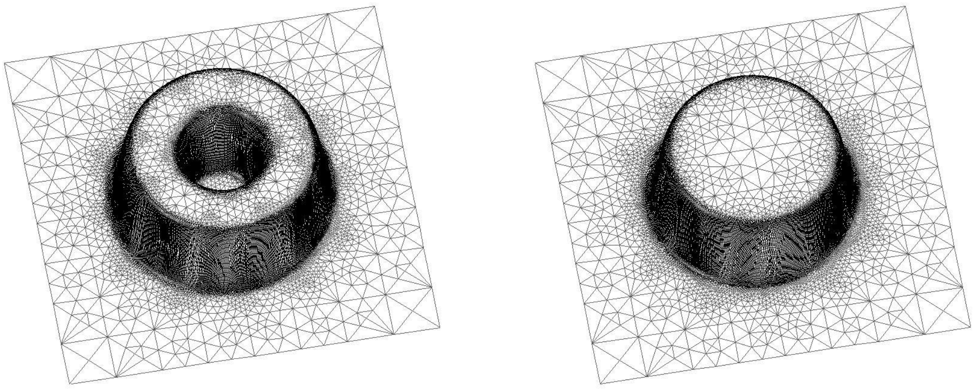

Figure 2: Experiment 1. Left: initial values; right: final state.

Experiment 1: We neglect elastic effects and consider the pure Cahn-Hilliard problem, i.e. $A = 0$. Let $r_1 = 0.55$ and $r_2 = 0.2$ and choose

$$\rho_0(x) = \min\Big(-\tanh\left(\tfrac{|x|-r_1}{\gamma\sqrt{2}}\right),\ \tanh\left(\tfrac{|x|-r_2}{\gamma\sqrt{2}}\right)\Big)\,.$$

Initially the interface consists of two concentric circles. Then the smaller circle shrinks until it vanishes completely and the solution reaches a stable state with only one circular interface, see Figure 2. In the sharp interface limit $\gamma \to 0$, the Ginzburg-Landau energy E from (1) converges to the interface length $2\pi|r_1(t) + r_2(t)|$ in the corresponding Mullins-Sekerka problem. Given this initial data, the Mullins-Sekerka problem can be reduced to a system of ordinary differential equations for the radii r_1 and r_2, cf. [4, 24]. Thereby we gain a reference solution to compare the accuracy of our numerical solution, see Figure 3.

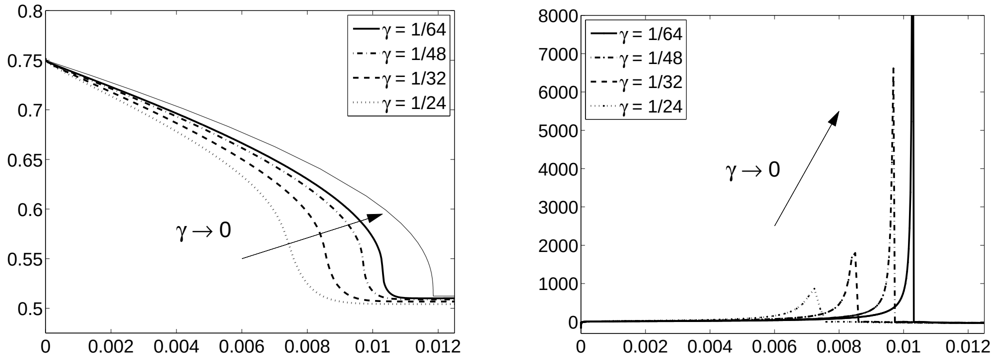

Figure 3: Left: Ginzburg-Landau energy $E(t)$ from (1) and interface length in the Mullins-Sekerka-Problem (thin solid line); right: numerically computed principal eigenvalue $-\Lambda(t)$.

When the inner interface vanishes, the system undergoes a topological change and the numerically computed principal eigenvalue $-\Lambda$ shows the predicted peak that grows proportionally to γ^{-1}, see Figure 3. The relation of the principal eigenvalue to the maximal interface curvature in the solution is illustrated in Figure 4. With decreasing parameter size γ, the interface thickness reduces and larger curvatures can be resolved.

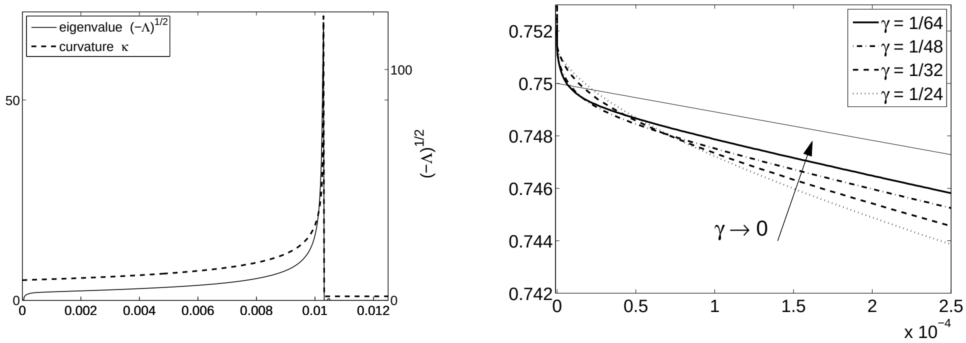

Figure 4: Experiment 1. Left: curvature of the inner interface in relation to the principal eigenvalue $-\Lambda$; right: the energy $E(t)$ indicates a rapid decay of perturbations in the initial values.

In the given experiment, the moving fronts of the solution show a self-similar profile across the interface. The chosen initial data ρ_0 does not perfectly match such a profile. Thus, the Ginzburg-Landau energy E is initially larger than the corresponding energy in the Mullins-Sekerka problem, but shows a fast relaxation during a time proportional to γ, see Figure 4.

6.2 Smooth Transition Layers After $T \sim \gamma$

In [22] it is stated that perturbations of a smooth transition layer between the bulk phases vanish within a time frame of order $O(\gamma)$. As long as there are no topological changes, the maximal interface curvature is uniformly bounded. The numerical experiments below confirm that this leads to a valid uniform upper bound for the principal eigenvalue $-\Lambda$.

Experiment 2: The initial configuration is given by a single circular interface

$$\rho_0(x) = -\tanh\left(\frac{|x| - r_1}{2\gamma\sqrt{2}}\right) ,$$

where the profile is flat compared to the final state in Example 1. During the time evolution, there are no other changes in the solution than a steepening of the interface profile to $-\tanh\left(\frac{|x|-r_1}{\gamma\sqrt{2}}\right)$.

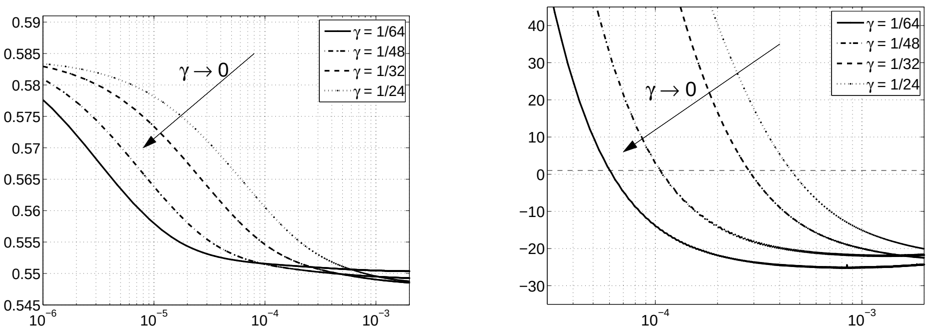

Figure 5: Experiment 2. Left: reduction of the Ginzburg-Landau energy $E(t)$; right: principal eigenvalue $-\Lambda(t)$.

From Figure 5 we see that within a time proportional to γ the initially large Ginzburg-Landau energy E reaches a lower level related to the final interface profile. As required by the error estimate, the principal eigenvalue $-\Lambda$ reduces to order $O(1)$ during a period $t \sim \gamma$.

When we prescribe initial values ρ_0 with a steep profile close to a jump, the principal eigenvalue initially takes large negative values, that are uncritical with respect to the error estimate. Again, $-\Lambda$ relaxes to order $O(1)$ within a time frame proportional to γ.

Experiment 3: The initial values take the form

$$\rho_0(x) = -\tanh\left(\frac{|x| - r_1}{\gamma\sqrt{2}}\right) + \text{noise} .$$

Here, the circular interface is perturbed by noise on a length scale between the mesh width h and the interface thickness γ, see Figure 6.

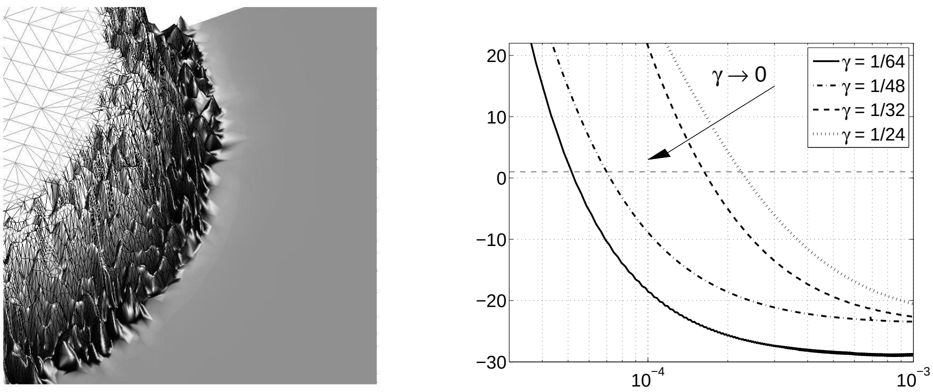

Figure 6: Experiment 3. Left: initial values; right: principal eigenvalue $-\Lambda(t)$.

As in Experiment 2, the numerical results confirm that the principal eigenvalue drops below an upper bound of order $O(1)$ within a time proportional to γ.

6.3 Application to Cahn-Larché System

Experiment 4: We choose the elasticity tensor to be of cubic symmetry by setting $\mathcal{C}_{1111} = \mathcal{C}_{2222} = 2$, $\mathcal{C}_{1122} = 1$ and $\mathcal{C}_{1212} = 20$. We set $\kappa = 0.1$ and choose initial values ρ_0 that describe two circular particles, where one is slightly larger than the other one. The radius of the larger particle is 1/6 whereas the radius of the other one is about 5.5% smaller. During the time evolution, the larger particle grows whereas the smaller one shrinks and is finally absorbed by the larger one by diffusion, see Figure 7.

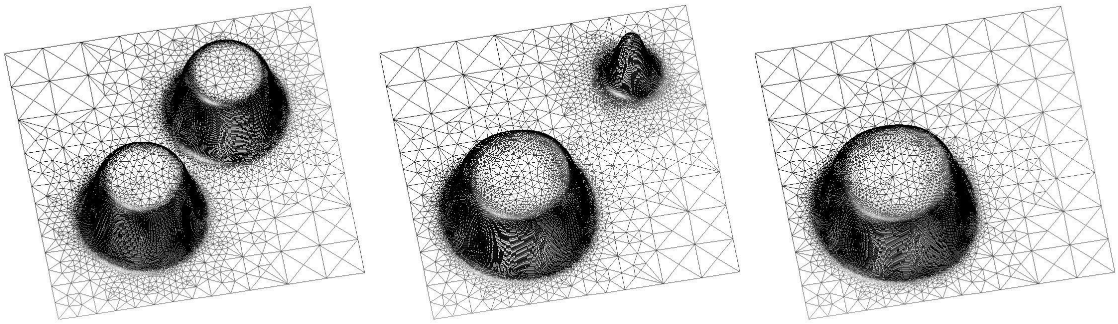

Figure 7: Experiment 4. Merging of two particles; snapshots of the solution ρ of the Cahn-Larché equation with homogeneous elasticity and $\gamma = 1/32$ are shown for $t = 0$, $t = 0.282$ and $t = 0.3$.

The numerical experiment underlines the importance to track the approximated principal eigenvalue. As required for the error control, $\Lambda(t)$ stays uniformly bounded with respect to γ^{-1} as long as there is no topological change in the solution and the critical point in time, when the smaller particle vanishes, is detected by a peak proportionally to γ^{-1}.

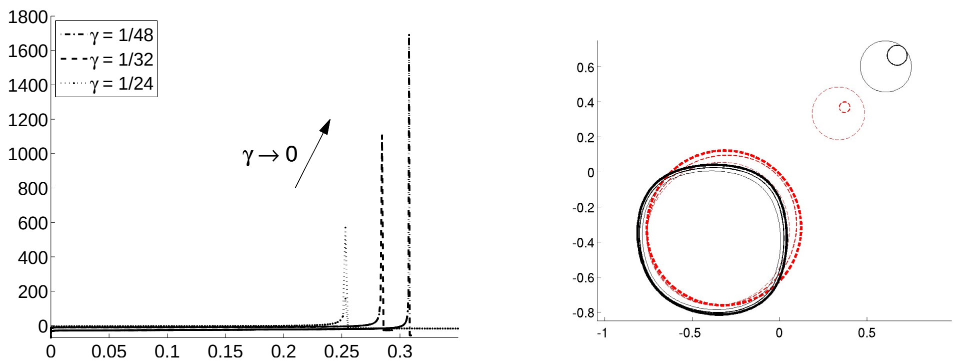

Figure 8: Experiment 4. Left: Numerically computed eigenvalues. The singularity reflects the topological change when the smaller particle vanishes; right: Comparison of the interface shape when elastic effects are neglected (dashed lines). Isolines $\rho^{(j)}(x) = 0$ are shown at times short before and after the vanishing of the smaller particle.

To illustrate the influence of the elasticity we compared the numerical solution with the results of a simulation where elasticity was neglected but all other parameters have been kept the same and the same initial data was used. Due to the anisotropy of the elasticity tensor the interface shows a more square like shape, compared to the pure Cahn-Hilliard case, where particles always develop a spherical shape. Moreover with elasticity included, the particles stay in a larger distance from each other, see Figure 8.

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