

Robust Error Estimates for Adaptive Phase Field Simulations

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Phase field equations are commonly used as a regularized model, where bulk phases are separated by interface regions that have a thickness of the order γ . Their numerical analysis is well established for a fixed parameter size γ , but conventional error estimates depend exponentially on γ^{-1} and thus become useless in the relevant case if $\gamma \rightarrow 0$. Technical applications include e. g. the simulation of Sn-Cu alloys for the production of lead free solder or Ni-Al alloys used for rotor blade surfaces.

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On a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, we consider the fourth order semilinear parabolic equation

$$\partial_t \rho - \Delta \left(-\gamma \Delta \rho + \frac{1}{\gamma} f(\rho) + \frac{1}{\gamma} A \rho \right) = 0. \quad (1)$$

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 and $f(\rho)$ is related to a smooth *double well potential*, that defines the stable states at $\rho = \pm 1$. The introduction of a general linear operator A is motivated by the modeling of elastic effects, that are neglected in the pure Cahn-Hilliard model, but become more and more important during the time evolution. To reduce the regularity requirements on the solution ρ , we introduce the *chemical potential* w defined as $w := -\gamma \Delta \rho + \gamma^{-1} (f(\rho) + A \rho)$.

Robust error estimates have been proved in [1,2] for the Allen-Cahn equation, that is closely related to (1) but only of second order. A priori estimates for the Cahn-Hilliard equation have been derived in [3]. A key argument is a spectral estimate, i.e. that the principal eigenvalue of the linearized operator about the exact solution is uniformly bounded with respect to γ , as long as no topological changes occur [4, 5]. Like proposed in [2], we use a linearization about the discrete approximate solution instead. Thereby we avoid a restriction on the initial data and gain the possibility to detect critical points in the time evolution. Then, for Cahn-Hilliard type equations like (1), one looks for the largest number λ and a function $q \neq 0$ such that

$$-\lambda q = \Delta \left(-\gamma \Delta q + \frac{1}{\gamma} f'(\hat{\rho}_h) q + \frac{1}{\gamma} A q \right). \quad (2)$$

As opposed to the case of the Allen-Cahn equation, we have to measure the error in the weaker H^{-1} norm. This makes it significantly harder to get control on a super-quadratic term in the error. At least for space dimension $d = 3$ we have to impose a growth condition on the potential function $f(\rho)$, that is satisfied, if $f \in C^{1,\delta}(\mathbb{R})$ and the derivative is Hölder continuous with exponent $0 < \delta < 1$. We have to derive computable a posteriori error bounds for the eigenvalue problem (2), that is also of fourth order. Moreover we have to take care about different constraints to the solution, the error of the equations and the eigenvalue problem. The following assumptions on the data 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 $\delta \in (0, 1)$ and $C_\delta \geq 0$, such that $-(b-a)(f(b) - f(a)) \leq -f'(b)(b-a)^2 + C_\delta |b-a|^{2+\delta}$ for all $a, b \in \mathbb{R}$.

(A3) $A : L^2(\Omega) \rightarrow L^2(\Omega)$ is linear selfadjoint and there is $\alpha > 0$, such that $-(\phi, A \phi) \leq \alpha \|\phi\|_{L^2(\Omega)}^2$ for all $\phi \in L^2(\Omega)$.

The quantities ρ and w are discretized with lowest order conforming finite elements. Let $0 = t_0 < t_1 < \dots < t_M = T$ be a partition of the time interval $[0, T]$. We consider shape regular meshes $\mathcal{T}^{(j)}$ without hanging nodes, which consist of simplicial elements. At time step j , the approximation space is denoted by $\mathcal{S}^{(j)} := \mathcal{S}(\mathcal{T}^{(j)})$. Using the notation $\bar{v} := \int_\Omega v \, dx$ for the meanvalue of a function, we define $\mathring{H}^1(\Omega) := \{v \in H^1(\Omega) : \bar{v} = 0\}$ and denote the subspace of finite element functions having meanvalue zero by $\mathring{\mathcal{S}}^{(j)}$.

Definition Let (ρ, w) be the exact solution of (1) with initial values $\rho(0, x) = \rho_0(x) \in H^1(\Omega)$ and natural boundary conditions and let (ρ_h, w_h) be a finite element approximation.

a) For almost all $s \in (0, T)$ the *residuals* $R_1(s)$ and $R_2(s)$ of the approximation (ρ_h, w_h) are defined as

$$\langle \phi, R_1 \rangle := (\nabla \phi, \nabla w_h) + \langle \phi, \partial_t \rho_h \rangle \quad \text{for all } \phi \in H^1(\Omega), \quad (3a)$$

$$\langle \psi, R_2 \rangle := \gamma (\nabla \psi, \nabla \rho_h) - (\psi, w_h) + \gamma^{-1} (\psi, f(\rho_h) + A \rho_h) \quad \text{for all } \psi \in H^1(\Omega). \quad (3b)$$

b) We define the *error* $e_1 := \rho_h - \rho - (\bar{\rho}_h - \bar{\rho}_0) := \mathring{e}_1 + \bar{e}_1$, with $\bar{e}_1 := \bar{\rho}_h - \bar{\rho}_0 \in \mathbb{R}$ and $\mathring{e}_1 \in \mathring{H}^1(\Omega)$.

c) The inverse Laplacian with natural boundary conditions $\Delta_N^{-1} : \mathring{H}^1(\Omega) \mapsto \mathring{H}^1(\Omega)$ is defined by $(\nabla \Delta_N^{-1} v, \nabla \phi) = -(v, \phi)$

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for all $\phi \in H^1(\Omega)$. Its discrete counterpart $\Delta_{N_h}^{-1} : \mathcal{S}^{(j)} \mapsto \mathring{\mathcal{S}}^{(j)}$ satisfies $(\nabla \Delta_{N_h}^{-1} v, \nabla \phi_h) = -(v, \phi_h)$ for all $\phi_h \in \mathcal{S}^{(j)}$. In the following we set $z := -\Delta_N^{-1} \mathring{e}_1$.

If we insert the exact solution (ρ, w) into (3), the residuals vanish and we recover the mixed variational formulation of the problem. Choosing $\phi = z$ and $\psi = \mathring{e}_1$ and combining the equations, we get the error equation

$$\frac{1}{2} \frac{d}{dt} \|\nabla z\|_{L^2(\Omega)}^2 + \gamma \|\nabla \mathring{e}_1\|_{L^2(\Omega)}^2 = \langle z, R_1 \rangle + \langle \mathring{e}_1, R_2 \rangle - \frac{1}{\gamma} (\mathring{e}_1, A \bar{e}_1) - \frac{1}{\gamma} (\mathring{e}_1, f(\rho_h) - f(\rho) + A \mathring{e}_1). \quad (4)$$

By introducing the Clément interpolant and using standard techniques we derive computable estimators η_1, η_{21} and η_{22} , such that $\langle \phi, R_1 \rangle \leq \eta_1 \|\nabla \phi\|_{L^2(\Omega)}$ and $\langle \psi, R_2 \rangle \leq \eta_{21} \|\nabla \psi\|_{L^2(\Omega)} + \eta_{22} \|\psi\|_{L^2(\Omega)}$. To control the nonlinear term containing $f(\rho)$, we need the principal eigenvalue λ and an a posteriori error estimator η_Λ , such that $-\Lambda^* := -\Lambda - \eta_\Lambda \leq -\lambda$ [6].

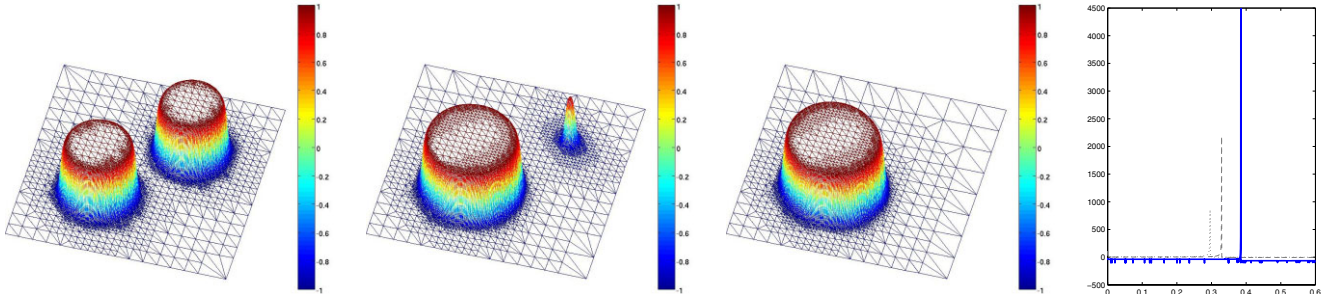


Fig. 1 Merging of two particles. Numerical solution obtained with $\gamma = \frac{1}{64}$ and corresponding numerical eigenvalue Λ over time t . The peak in the eigenvalue reflects the topological change in the solution when the smaller particle vanishes. The dotted line shows the eigenvalue for $\gamma = \frac{1}{16}$ and dashed line for $\gamma = \frac{1}{32}$.

Definition Let (λ, q) be the solution of (2) and (Λ, q_h) an approximation thereof. The residual R_Λ is defined by

$$\langle v, R_\Lambda \rangle := \Lambda (v, \Delta_N^{-1} q_h) - \gamma (\nabla v, \nabla q_h) - \gamma^{-1} (v, f'(\hat{\rho}_h) q_h) - \gamma^{-1} (v, A q_h) \text{ for all } v \in H^1(\Omega). \quad (5)$$

Again by inserting the exact eigenvalue-eigenfunction pair into (5), the residual R_Λ vanishes and we recover the weak form of the eigenvalue problem. For the error in the eigenvalue we have the identity $\Lambda - \lambda = \langle P_\lambda q_h, R_\Lambda \rangle / (P_\lambda q_h, \Delta_N^{-1} q_h)$. Although in general it is not clear, that the denominator is bounded away from 0, it is quite common to make the following *saturation assumption* $\|\nabla \Delta_N^{-1} (q_h - P_\lambda q_h)\|_{L^2(\Omega)}^2 \leq \frac{1}{2}$, i.e. to assume that the approximate eigenvalue is sufficiently close to the eigenspace of the continuous problem. In consequence we get $(P_\lambda q_h, \Delta_N^{-1} q_h) \leq -\frac{1}{8}$.

Theorem ([6]) Let P_λ be the L^2 projection to the subspace related with the principal eigenvalue λ . Let (Λ, q_h) be the approximative solution of the discrete eigenvalue problem with $\|\nabla \Delta_{N_h}^{-1} q_h\|_{L^2(\Omega)} = 1$. Let η_A and η_{N_h} be computable estimators for the residuals due to the approximation of A and Δ_N^{-1} , respective. Then, we have

$$\lambda - \Lambda \leq 8\gamma^{-1/2} (\eta_{q_h} + \eta_A) \left((\|f'(\hat{\rho}_h)\|_\infty + \alpha) \|q_h\|^2 - \Lambda (\eta_{N_h} + 3/2) \right)^{1/2} + 8\Lambda (\eta_{N_h} + 3/2) \eta_{N_h}. \quad (6)$$

Then the proof of the following robust a posteriori error estimate is established by a continuation argument [6].

Theorem ([6]) Let $\gamma < 1$ and $\frac{5}{7} < \delta \leq \frac{4}{5}$. There are constants $\mu_1, \mu_2 \sim e^{-2\Lambda^* T}$ independent of γ , such that given a tolerance $\theta \leq \gamma^7 \mu_1 < 1$ and suppose the approximation error of the initial values and the residual estimate can be controlled by this tolerance θ , i.e. $\|\nabla \Delta_N^{-1} (\rho_h^{(0)} - \rho_0)\|_{L^2(\Omega)}^2 \leq \mu_2 \theta^2$ and $\int_0^T \eta^2 ds \leq \mu_2 \theta^2$. Then, we have

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

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