Numerical analysis for phase field simulations of moving interfaces with topological changes

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Phase field methods are a widely accepted tool for the approximation of moving free interfaces in sharp interface problems. Topological changes in the solution, such as nucleation or vanishing of particles or merging or pinching of interfaces, lead to singularities in the free boundary. In the sharp interface model, these singularities cause both numerical and theoretical problems, whereas they are handled "automatically" in phase field simulations. Phase field models contain a length scale $\varepsilon > 0$ that vanishes in the sharp interface limit. Therefore, when $\varepsilon \to 0$, practical numerical methods have to be robust in the sense that error estimates may only depend polynomially on ε^{-1}, not exponentially. We show that robust error control is possible past the occurrence of topological changes and without restrictive assumptions on the initial data.

1 Problem Formulation

For brevity of the presentation, we only consider the Allen-Cahn equation here, but remark that analogous results hold for complex valued Ginzburg-Landau equations, fourth order Cahn-Hilliard equations and Cahn-Larché equations with linear elasticity [2–4]. Let $\Omega \subset \mathbf{R}^d$, $d = 2, 3$ be a Lipschitz domain and $T > 0$ a time horizon. Given $u(0, \cdot) = u_0 \in H^1(\Omega)$, in the weak form of the problem, we have to find $u \in L^2(0, T, H^1(\Omega) \cap H^1(0, T, (H^1(\Omega))^*)$ such that for almost all $t \in [0, T]$

$$\langle \phi, \partial_t u \rangle + \big(\nabla \phi, \nabla u\big) + \varepsilon^{-2}\big(\phi, f(u)\big) = 0 \quad \text{for all } \phi \in H^1(\Omega)\,. \tag{1}$$

Here, f is a nonlinear function related to a smooth double well potential, e. g. $f(u) = (u^2 - 1)u$. More general, we impose the following assumptions: there are $0 < C_f$, $0 < \delta \leq 1$ and a non-negative function $g \in C(\mathbf{R})$ such that for all $\phi, \psi \in H^1(\Omega)$

$$-f' \leq C_f, \qquad -\big(\phi - \psi, f(\phi) - f(\psi)\big) \leq -\big(\phi - \psi, f'(\phi)(\phi - \psi)\big) + g(\phi)\|\phi - \psi\|^{2+\delta}_{L^{2+\delta}(\Omega)}\,. \qquad \text{(A1), (A2)}$$

Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a partition of the time interval. At each time level t_j, we introduce a shape regular triangulation $\mathcal{T}^j$ of Ω and denote by $\mathcal{S}^1(\mathcal{T}^j)$ the space of lowest order conforming finite elements. Then, the fully discrete problem consists of a numerical scheme to determine the approximate solution $\{u_h^j \in \mathcal{S}^1(\mathcal{T}^j) : 0 \leq j \leq N\}$. Examples of suitable numerical schemes are given in [1, 3, 7], but we would like to stress that the abstract a posteriori analysis presented below requires no assumptions on how the approximate solution was obtained.

2 Abstract a Posteriori Error Analysis

Let $u_h^j \in \mathcal{S}^1(\mathcal{T}^j), 0 \leq j \leq N$, be arbitrary finite element functions and denote by u_h the piecewise affine interpolation with respect to time. Let u be the weak solution of (1) and define the *error* $e := u_h - u$. For almost all $t \in [0, T]$, we define *residual* R and choose the quantities η_0, η_1 such that

$$(\phi, \partial_t u_h) + (\nabla \phi, \nabla u_h) + \varepsilon^{-2}(\phi, f(u_h)) =: \langle \phi, R \rangle \quad \leq \eta_0\|\phi\| + \eta_1\|\nabla \phi\| \quad \text{for all } \phi \in H^1(\Omega). \tag{2}$$

Possibly, fully computable choices of η_0, η_1 for semi-implicit numerical schemes are given in [1, 3, 7]. Subtracting (1) from the residual in (2) and choosing $\phi = e$, we get an evolution equation for the error

$$\tfrac{1}{2}\tfrac{d}{dt}\|e\|^2 + \|\nabla e\|^2 = \langle e, R \rangle - \varepsilon^{-2}(e, f(u_h) - f(u))\,. \tag{3}$$

From (3), we derive two different inequalities. With (A1) and the residual estimator $\tilde{\eta}^2 := \varepsilon^2\eta_0^2/(4C_f) + \eta_1^2/2$, we get

$$\tfrac{1}{2}\tfrac{d}{dt}\|e\|^2 + \|\nabla e\|^2 \leq \eta_0\|e\| + \eta_1\|\nabla e\| + \varepsilon^{-2}C_f\|e\|^2 \quad \leq \tilde{\eta}^2 + \tfrac{1}{2}\|\nabla e\|^2 + \varepsilon^{-2}2C_f\|e\|^2\,. \tag{4}$$

Due to the coefficient ε^{-1} in front of the last term on the right hand side, a direct application of Gronwall's lemma would lead to a useless error bound that grows exponentially in ε^{-1}. In Phase field models, sharp interfaces are approximated by fronts

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of width $\mathcal{O}(\varepsilon)$ where the solution u has a slope of order ε^{-1}. This suggests that the terms on the left hand side of (4) are of different order in ε^{-1}, i. e. $\|\nabla e\|^2/\|e\|^2 \sim \varepsilon^{-2}$ and that a pure L^2–error estimate should be possible without the exponential dependence on ε^{-1}. With (3) and (A2), we estimate

$$\tfrac{1}{2}\tfrac{d}{dt}\|e\|^2 \le \langle e, R\rangle - \frac{\|\nabla e\|^2}{\|e\|^2}\|e\|^2 - \varepsilon^{-2}\big(e, f'(u_h)e\big) + \varepsilon^{-2}g(u_h)\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)} \le \langle e, R\rangle + \Lambda\|e\|^2 + \varepsilon^{-2}g(u_h)\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)},$$

where Λ is the principal eigenvalue of linearized Allen-Cahn operator at the approximate solution u_h

$$-\Lambda := \inf_{q\in H^1(\Omega)\setminus 0} \frac{\|\nabla q\|^2 + \varepsilon^{-2}(q, f'(u_h)q)}{\|q\|^2}. \tag{5}$$

To retrieve control of $\|\nabla e\|$, we add to the above inequality a small portion of the coarse estimate (4), weighted by a factor up to ε^2. Then, there are a constant $\Lambda_0 > 0$ and a residual estimator η such that

$$\tfrac{1}{2}\tfrac{d}{dt}\|e\|^2 + \tfrac{1}{2}\varepsilon^2\|\nabla e\|^2 \le \eta^2 + (\Lambda_0 + \Lambda)\|e\|^2 + \varepsilon^{-2}g(u_h)\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)}.$$

Because of the term containing $\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)}$, we have to apply a generalized Gronwall lemma [3] leading to an error estimate with an extra condition on the smallness of the residuum: if $\eta^2 \le \varepsilon^4 C_1 \exp\big(-8\int_0^T 2\max(0,\Lambda_0+\Lambda)\,\mathrm{d}s\big)$ then

$$\sup_{t\in[0,T]} \|e(t)\|^2 + \varepsilon^2\int_0^T \|\nabla e\|^2\,\mathrm{d}s \le 8\eta^2 \exp\big(\int_0^T 2\max(0,\Lambda_0+\Lambda)\,\mathrm{d}s\big). \tag{6}$$

3 Robust Error Control Past Topological Changes

The form of (6) is typical in the context of robust error control for more general phase field models. It has no explicit exponential dependence on ε^{-1} but contains an expression involving the principle eigenvalue. The importance of appropriate bounds for Λ has already been noticed in [5]. First robust a priori estimates for the Allen-Cahn equation (1) have been developed in [6] and a posteriori error estimates were given in [7]. They are based on analytical results providing for $\varepsilon \to 0$ uniform bounds for the principal eigenvalue λ of the linearized operator at the exact solution u. These bounds require that the phase field has developed a smooth profile across interfaces, leading to restrictive assumptions on the initial data. Moreover, they break down when topological changes occur, and in general it is not possible to predict these singularities in advance. For Cahn-Larché equations or other more complicated situations, there is no uniform spectral estimate available so far.

We take the slightly different approach proposed in [1] and follow the philosophy outlined in [5] to "replace as much as possible 'analytical knowledge' ...with 'computational knowledge' ". Numerical evidence shows [2–4] that topological changes for which $\Lambda(t) \approx \lambda(t) \sim \varepsilon^{-2}$ occur within temporal intervals of length comparable to ε^2 leading to

$$\int_0^T \max(0,\Lambda(s))\,ds \le C + \ln\varepsilon^{-\alpha}, \tag{7}$$

what is sufficient for robust a posteriori error analysis based on (6). Moreover, by the numerical computation of Λ, it is possible to determine critical times where robust error estimation breaks down and we are able to assess the stability of the simulated phase field model against singularities that might cause large deviations of the evolution with $\varepsilon > 0$ from the sharp interface limit. The numerical experiments also show that initial perturbations of an interface relax sufficiently fast to allow a uniform bound for the time-integrated eigenvalue Λ. Thereby, the restrictions on the initial data are removed.

Since this a posteriori estimates depend on the numerical solution of eigenvalue problem, we also have to control numerical errors within this subproblem. Suitable a posteriori and a priori error estimates for the eigenvalue problem are derived in [1–3].

In light of the numerical experiments, it is reasonable to assume a bound of the form (7) for the principal eigenvalue λ. Then, in a slight modification of [6], we get robust a priori error control past topological changes, see [3]. This in turn makes an analytical proof of (7) highly desirable, at least in some simple prototypical situations.

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