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Robust a-posteriori error control of Cahn-Hilliard type equations with elasticity

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Phase separation of an initially homogeneous mixture into two different phases can be modeled on a mesoscopic scale by the Cahn-Hilliard equation. The interface thickness between the pure phases enters as a small parameter γ into this mass conserving fourth order semilinear parabolic equation. Numerical analysis is well established for a fixed parameter size, but error estimates depend exponentially on γ^{-1} and thus become useless if $\gamma \to 0$. We consider the case, that elastic stresses due to a lattice misfit become important and the equation has to be coupled to a system of linear elasticity. 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.

Let the bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be occupied by the alloy. At each point $x \in \Omega$ the state of the alloy is given by the difference $\rho \in [-1, 1]$ between the volume fractions. The *chemical potential* w is defined as $w := -\gamma\Delta\rho + \frac{1}{\gamma} f(\rho)$, where A is the linear operator related to elasticity and $f(\rho)$ is the derivative of a *double well potential* $\mathcal{F}(\rho)$. The most common example of a continuous potential is $\mathcal{F}(\rho) := (\rho^2 - 1)^2$. The Cahn-Hilliard equation with homogenous elasticity can be written in the form $\partial_t\rho = \Delta(-\gamma\Delta\rho + \frac{1}{\gamma} f(\rho) + \frac{1}{\gamma} A\,\rho)$ and the pure Cahn-Hilliard equation is recovered if $A = 0$. In a mixed variational formulation the problem reads: given an initial configuration $\rho(0, x) = \rho_0(x) \in H^1(\Omega)$, find $(\rho, w) \in H^1\left([0, T], H^1(\Omega)\right) \times L^\infty\left([0, T], H^1(\Omega)\right)$, such that for almost all $t \in (0, T)$

$$0 = \langle \phi, \partial_t\rho \rangle + (\nabla\phi, \nabla w) \qquad \text{for all } \phi \in H^1(\Omega)\,, \tag{1a}$$

$$0 = \gamma\,(\nabla\psi, \nabla\rho) - (\psi, w) + \tfrac{1}{\gamma}\,(\psi, f(\rho) + A\rho) \qquad \text{for all } \psi \in H^1(\Omega)\,. \tag{1b}$$

Robust a-posteriori error estimates for similar, but second order nonconservative Allen-Cahn and Ginzburg-Landau problems have been achieved by using a spectral argument [5, 1]. They are based on the observation that the principal eigenvalue of the linearized operator is bounded, as long, as no topological changes in the solution occur. The same holds true for the Cahn-Hilliard equation [2, 3] and has been used for an a-priori analysis that is robust with respect to γ, see [4]. In our case of the Cahn-Hilliard equation with homogenous elasticity, the principal eigenvalue is

$$-\lambda := \inf_{\substack{v \in \mathring{H}^1(\Omega) \\ -\Delta y = v}} \frac{\gamma\,\|\nabla v\|^2_{L^2(\Omega)} + \frac{1}{\gamma}\,(v, f'(\rho_h)v + A\,v)}{\|\nabla y\|^2_{L^2(\Omega)}}\,. \tag{2}$$

1 Finite Element Setting

We subdivide the time interval $[0, T]$ into N timesteps of size $\tau_j := t_j - t_{j-1}$, $j = 1, \cdots, N$. At each time level t_j, let $\mathcal{T}^{(j)}$ be a shape regular triangulation of Ω and $\mathcal{S}^1(\mathcal{T}^{(j)})$ the space of conforming first order finite elements. The nodal interpolation operator on $\mathcal{T}^{(j)}$ is denoted by $\mathcal{I}_{\mathcal{T}^{(j)}}$. Using a backward Euler discretization with respect to time, we apply for $j = 1, \cdots, N$ the numerical scheme

$$\left(\phi_h, \rho_h^{(j)}\right) + \tau_j\left(\nabla\phi_h, \nabla w^{(j)}\right) = \left(\phi_h, \mathcal{I}_{\mathcal{T}_j}\rho_h^{(j-1)}\right) \qquad \text{for all } \phi_h \in \mathcal{S}^1(\mathcal{T}^{(j)}), \tag{3a}$$

$$\left(\psi_h, w^{(j)}\right) - \gamma\left(\nabla\psi_h, \nabla\rho_h^{(j)}\right) = \tfrac{1}{\gamma}\left(\psi_h, f(\mathcal{I}_{\mathcal{T}_j}\rho_h^{(j-1)}) + A_h\rho_h^{(j-1)}\right) \qquad \text{for all } \psi_h \in \mathcal{S}^1(\mathcal{T}^{(j)}), \tag{3b}$$

where A_h is an approximation of the linear operator A due to finite element solution of the elasticity problem. Afterwards, continuous in time solutions ρ_h and w_h are defined by piecewise affine interpolation between the time levels t_j.

Definition 1.1 a) For $v \in H^1(\Omega)$ the *meanvalue* is $\bar{v} := \frac{1}{|\Omega|}\int_\Omega v\,dx$, and we define $\mathring{H}^1(\Omega) := \{v \in H^1(\Omega) : \bar{v} = 0\}$.
b) Let (ρ, w) be the solution of (1) and (ρ_h, w_h) a finite element approximation. The *error* is $e := \rho_h - \rho - (\bar{\rho}_h - \bar{\rho}) \in \mathring{H}^1(\Omega)$. Furthermore we set $z \in \mathring{H}^1(\Omega)$ to be the solution of $-\Delta z = e$, with natural boundary conditions $\partial_{\vec{n}} z = 0$ on $\partial\Omega$.
c) For almost all $s \in (0, T)$ the *residuals* $R_1(s),\ R_2(s)$ of the approximation (ρ_h, w_h) are defined as

$$\langle \phi, R_1(s) \rangle := \langle \phi, \partial_t\rho_h \rangle + (\nabla\phi, \nabla w_h) \qquad \text{for all } \phi \in H^1(\Omega)\,, \tag{4a}$$

$$\langle \psi, R_2(s) \rangle := \gamma\,(\nabla\psi, \nabla\rho_h) - (\psi, w_h) + \tfrac{1}{\gamma}\,(\psi, f(\rho_h) + A_h\rho_h) \qquad \text{for all } \psi \in H^1(\Omega)\,. \tag{4b}$$

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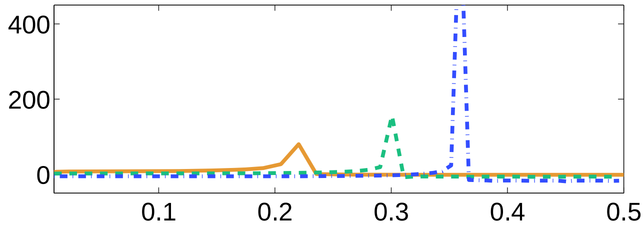

Fig. 1 Merging of two particles. Top row: Solution obtained by numerical simulation with $\gamma = \frac{1}{24}$. Left: Corresponding eigenvalue λ_h over time t, computed numerically for different parameter sizes $\gamma = \frac{1}{16}$ (solid line), $\gamma = \frac{1}{24}$ (dashed line) and $\gamma = \frac{1}{32}$.

Subtracting the equations (1) from the residuals (4) and choosing $\phi = z$ and $\psi = e$, we can derive the error equation

$$\tfrac{1}{2}\tfrac{d}{dt}\|\nabla z\|^2_{L^2(\Omega)} + \gamma\|\nabla e\|^2_{L^2(\Omega)} = \langle z, R_1\rangle + \langle e, R_2\rangle - \tfrac{1}{\gamma}\left(e, f(\rho_h) - f(\rho)\right) - \tfrac{1}{\gamma}\left(e, A_h\,\rho_h - A\,\rho\right) . \qquad (5)$$

2 A-Posteriori Error Estimate

With standard techniques and referring to [6] for the elasticity part, we can estimate the residuals.

Lemma 2.1 *There are a computable residual estimator η and constants μ_1, mu_2, μ_1 uniformly bounded with respect to γ^{-1} and $\mu_2 \le \frac{1}{4}$, such that*

$$\langle z, R_1\rangle + \langle e, R_2\rangle - \tfrac{1}{\gamma}\left(e, (A_h - A)\rho_h\right) \le \eta^2 + \mu_1\|\nabla z\|^2_{L^2(\Omega)} + \mu_2\gamma^4\|\nabla e\|^2_{L^2(\Omega)} .$$

To control the nonlinearity in (5), we use a spectral estimate, involving the eigenvalue given in (2), but we also have to take a convex combination with a ”coarser estimate”, weighted by the factor γ^3.

Lemma 2.2 *Assume $f \in C^1(\mathbb{R})$ and there are constant $\delta \in (0,1)$ and $C_\delta,\ C_f > 0$ such that almost everywhere $-f' \le C_f$ and $e\left(f(\rho) - f(\rho_h)\right) \le -f'(\rho_h)e^2 + C_\delta|e|^{2+\delta}$. Let λ be according to (2) and set $\Lambda_1 := \mu_1 + \lambda + \frac{1}{2}C_f^2$. Then there holds*

$$\tfrac{1}{2}\tfrac{d}{dt}\|\nabla z\|^2_{L^2(\Omega)} + \tfrac{1}{4}\gamma^4\|\nabla e\|^2_{L^2(\Omega)} \le \eta^2 + \Lambda_1\|\nabla z\|^2_{L^2(\Omega)} + \tfrac{1}{\gamma}C_\delta\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)} . \qquad (6)$$

Now we have to carefully estimate the last term in (6) in such a way, that after applying a Sobolev inequality we gain sufficient large extra powers of ∇z. Then by a continuation argument we can show the following result

Theorem 2.3 *Let $\gamma < 1$ and $\frac{5}{7} < \delta \le \frac{4}{5}$. Assume that for $t \in [0,T]$ the eigenvalue λ is uniformly bounded with respect to γ^{-1}. Set $C_1 := \exp(-2\Lambda_1 T)/6$ and $C_2 \sim C_1^{7/5}$ up to a factor depending only on the space dimension $d = 2, 3$ and the domain $\Omega \subset \mathbb{R}^d$. Given a tolerance $\theta \le \gamma^7 C_2 < 1$, suppose the initial values $\|\nabla z_0\|^2_{L^2(\Omega)} \le C_1\theta^2$ and the residual estimate can be controlled by $\int_0^T \eta^2\,ds \le C_1\theta^2$, then*

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

Instead of assuming a uniform bound for the principal eigenvalue λ, the numerical computation of the approximative eigenvalue λ_h in each timestep leads to a fully computable error control. Moreover, one thereby gains the possibility to detect critical points in the solution, like topological changes. In Figure 1 it is shown, that the vanishing of a particle is associated with a peak in the eigenvalue λ_h and there is no bound upper on the height of the peaks.

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