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DEGENERATE AREA PRESERVING SURFACE ALLEN–CAHN EQUATION AND ITS SHARP INTERFACE LIMIT

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Abstract. We consider formal matched asymptotics to show the convergence of a degenerate area preserving surface Allen–Cahn equation to its sharp interface limit of area preserving geodesic curvature flow. The degeneracy results from a surface de Gennes–Cahn–Hilliard energy and turns out to be essential to numerically resolve the dependency of the solution on geometric properties of the surface. We experimentally demonstrate convergence of the numerical algorithm, which considers a graph formulation, adaptive finite elements and a semi-implicit discretization in time, and uses numerical solutions of the sharp interface limit, also considered in a graph formulation, as benchmark solutions. The results provide the mathematical basis to explore the impact of curvature on cells and their collective behaviour. This is essential to understand the physical processes underlying morphogenesis.

Key words. Motion by geodesic curvature, surface Allen–Cahn equation, de Gennes–Cahn–Hilliard energy, matched asymptotic expansion, graph formulation.

1. Introduction

The connection between phase field approximations and geometric partial differential equations is well established and can formally be justified by matched asymptotics, see [1]. Geometric partial differential equations are evolution equations that evolve curves or surfaces according to their curvature. Prominent examples are mean curvature flow, area preserving mean curvature flow or surface diffusion, see [2, 3] for reviews. Similarly to these curvature driven flows in 2D or 3D one can consider the evolution of curves on surfaces. The evolution of these curves is governed by geodesic curvature and thus strongly depends on the local geometric properties of the underlying surface. First analytical attempts to connect these geodesic evolution laws to surface phase field models have been considered in [4, 5, 6, 7]. We here show this connection for a degenerate area preserving surface Allen–Cahn equation and an area preserving geodesic curvature flow.

This model is of particular interest in mathematical biology, where it is used to approximate cells in epithelial tissue [8, 9, 10]. These approaches are considered in 2D. Their extension to surfaces provides the mathematical basis to explore the impact of curvature on cells and their collective behaviour. This is essential to understand the physical processes underlying morphogenesis. First attempts in this direction [11, 12] show a huge impact of curvature on collective motion but also the sensitivity of the solution on local geometric properties of the surface, which asks for further mathematical foundations to which this paper contributes.

2. Mathematical models

We consider a surface de Gennes–Cahn–Hilliard energy

$$\mathcal{F}_{dGCH}(\phi) = \tilde{\sigma} \int_{\mathcal{S}} \frac{1}{G(\phi)} \left(\frac{\epsilon}{2} \|\nabla_{\mathcal{S}} \phi\|^2 + \frac{1}{\epsilon} W(\phi) \right) d\mathcal{S} \tag{1}$$

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with surface $\mathcal{S}$, phase field variable ϕ, surface gradient $\nabla_{\mathcal{S}}$, double well potential $W(\phi) = \frac{1}{4}(\phi^2-1)^2$, rescaled surface tension $\tilde{\sigma}$ and small parameter $\epsilon > 0$ determining the thickness of the diffuse interface. The factor $1/G(\phi)$ is called the de Gennes coefficient in polymer science. We consider $G(\phi) = \frac{3}{2}(1-\phi^2)$ or a regularized version $G_\eta(\phi) = (\frac{9}{4}(1-\phi^2)^2 + \eta^2\epsilon^2)^{1/2}$ with $\eta > 0$. The scaling coefficient is such that the sharp interface limit equals the one obtained from the usual Cahn–Hilliard energy without the de Gennes coefficient [13, 14]. Evolution equations based on this energy, at least in 2D and 3D, have been shown numerically advantageous, as the singularity, $G(\phi)$ or $G_\eta(\phi)$, helps to keep solutions confined in $[-1, 1]$. However, a theoretical foundation of this argument remains open. From a practical point of view, the de Gennes coefficient allows to achieve the same accuracy with larger ϵ. Several numerical studies use this to achieve results which would not be possible without it, see [15, 16]. We will demonstrate that this advantage is also present on surfaces and becomes essential to numerically resolve the dependency of the solution on geometric properties of the surface.

The L^2-gradient flow of eq. (1) on $\mathcal{S}$ with an appropriate scaling in time reads

$$\begin{aligned}\epsilon\tilde{\beta}\partial_t\phi &= \tilde{\sigma}\left(\epsilon\nabla_{\mathcal{S}}\cdot\left(\frac{1}{G(\phi)}\nabla_{\mathcal{S}}\phi\right) - \frac{1}{\epsilon G(\phi)}W'(\phi)\right)\\ &\quad - \tilde{\sigma}\left(\frac{1}{G(\phi)}\right)'\left(\frac{\epsilon}{2}\|\nabla_{\mathcal{S}}\phi\|^2 + \frac{1}{\epsilon}W(\phi)\right),\end{aligned}$$

with surface divergence $\nabla_{\mathcal{S}}\cdot$ and Laplace–Beltrami operator $\Delta_{\mathcal{S}}$. $\tilde{\beta} > 0$ is a rescaled kinetic coefficient. Using the asymptotic approximation [17] $\frac{\epsilon}{2}\|\nabla_{\mathcal{S}}\phi\|^2 \approx \frac{1}{\epsilon}W(\phi)$ and the identity $\nabla_{\mathcal{S}}\cdot((1/G(\phi))\nabla_{\mathcal{S}}\phi) = (1/G(\phi))\,\Delta_{\mathcal{S}}\phi + (1/G(\phi))'\,\|\nabla_{\mathcal{S}}\phi\|^2$ we can approximate this equation by

$$\epsilon\tilde{\beta}\partial_t\phi = \frac{\tilde{\sigma}}{G(\phi)}\left(\epsilon\Delta_{\mathcal{S}}\phi - \frac{1}{\epsilon}W'(\phi)\right). \tag{2}$$

The idea for this approximation was first used for phase field approximations of surface diffusion in [18], where $G(\phi)$ was introduced as a stabilizing function. Due to this approximation the gradient flow structure is lost. However, the computational cost is comparable to the formulation without $G(\phi)$. For a detailed derivation and numerical comparison of the full and the approximated formulation in 2D, see [13].

We now introduce the Lagrange multiplier λ in eq. (2) to ensure the area constraint $1/|\mathcal{S}|\int_{\mathcal{S}}\phi\, d\mathcal{S} = \alpha$ with $\alpha \in [-1, 1]$. The resulting system reads

$$\epsilon\tilde{\beta}\partial_t\phi = \frac{\tilde{\sigma}}{G(\phi)}\left(\epsilon\Delta_{\mathcal{S}}\phi - \frac{1}{\epsilon}W'(\phi)\right) + \lambda \tag{3}$$

$$\frac{1}{|\mathcal{S}|}\int_{\mathcal{S}}\phi\, d\mathcal{S} = \alpha. \tag{4}$$

By integrating eq. (3) over $\mathcal{S}$, and inserting the time derivative of eq. (4), we obtain

$$0 = \tilde{\sigma}\int_{\mathcal{S}}\frac{1}{G(\phi)}\left(\epsilon\Delta_{\mathcal{S}}\phi - \frac{1}{\epsilon}W'(\phi)\right) d\mathcal{S} + |\mathcal{S}|\lambda.$$

By solving for λ we arrive at the equation to be considered, a degenerate area preserving surface Allen–Cahn equation on $\mathcal{S}$

$$\epsilon\tilde{\beta}G(\phi)\partial_t\phi = \tilde{\sigma}\left(\epsilon\Delta_{\mathcal{S}}\phi - \frac{1}{\epsilon}W'(\phi)\right) + G(\phi)\lambda, \tag{5}$$

$$\lambda = \tilde{\sigma}\frac{1}{|\mathcal{S}|}\int_{\mathcal{S}}\left(-\frac{\epsilon}{G(\phi)}\Delta_{\mathcal{S}}\phi + \frac{1}{\epsilon G(\phi)}W'(\phi)\right) d\mathcal{S}, \tag{6}$$