INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 16, Number 2, Pages 192–209

CONVEXITY SPLITTING IN A PHASE FIELD MODEL FOR SURFACE DIFFUSION

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Abstract. Convexity splitting like schemes with improved accuracy are proposed for a phase field model for surface diffusion. The schemes are developed to enable large scale simulations in three spatial dimensions describing experimentally observed solid state dewetting phenomena. We carefully elaborate the loss in accuracy associated with large time steps in such schemes and show the existence of a maximal numerical timestep to achieve a prescribed accuracy. We demonstrate the increase of this maximal numerical time step by at least one order of magnitude using a Rosenbrock method. This convexity splitting scheme with improved accuracy is used to study the effect of contact angle on solid state dewetting phenomena.

Key words. Convexity splitting, Rosenbrock time discretization, surface diffusion, solid-state dewetting.

1. Introduction

If an energy $\mathcal{E}$ can be written as the difference of two convex energies $\mathcal{E}_c$ and $\mathcal{E}_e$, $\mathcal{E} = \mathcal{E}_c - \mathcal{E}_e$, then the time discretization

$$\frac{u^{n+1} - u^n}{\tau_n} = -\nabla_{\mathcal{H}} \mathcal{E}_c[u^{n+1}] - \nabla_{\mathcal{H}} \mathcal{E}_e[u^n]$$

of the gradient flow

$$u_t = -\nabla_{\mathcal{H}} \mathcal{E}[u]$$

is energy stable. That is, it satisfies $\mathcal{E}[u^{n+1}] \leq \mathcal{E}[u^n]$ for all time steps n. Here, $\tau_n = t^{n+1} - t^n$ is the discrete time step width, u^n denotes the time-discrete approximation of $u(t^n)$, $\nabla_{\mathcal{H}} \mathcal{E}$ denotes the gradient of an energy $\mathcal{E}$ with respect to the inner product of a Hilbert space $\mathcal{H}$, defined by $(\nabla_{\mathcal{H}} \mathcal{E}[u], \theta)_{\mathcal{H}} = \delta_u \mathcal{E}[u](\theta)$ for all $\theta \in \mathcal{H}$, where the right-hand side is the Gateaux derivative of $\mathcal{E}$ in a test function θ. Typical choices are $\mathcal{H} = L^2$, for non-conserved flows, and $\mathcal{H} = H^{-1}$, for conserved flows. This convexity splitting idea is often attributed to Eyre [18] and has become popular as a simple and efficient discretization scheme for various evolution problems with a gradient flow structure, see e.g. [10, 59, 20, 17, 54, 48, 49]. Some of these schemes are shown to be unconditionally energy stable, unconditionally solvable and converge optimally in the energy norm. However, it has also been shown that convexity splitting approaches can lead to large errors [10, 11, 17, 19]. We will elaborate on this issue and propose a convexity splitting approach for a phase field model for surface diffusion with improved accuracy.

The model to be considered reads [42]

$$\partial_t u = \nabla \cdot \mathbf{j}, \qquad \mathbf{j} = \frac{1}{\epsilon} M(u) \nabla \mu, \qquad g(u)\mu = \frac{1}{\epsilon} B'(u) - \epsilon \Delta u, \tag{1}$$

in $\Omega \times (0, \infty)$ with $\Omega \subset \mathbb{R}^d$ with $d = 2, 3$. The variable u denotes an order parameter for the phases of the system, such that, for example, $u = 1$ represents a solid phase, and $u = 0$ represents a liquid phase. The variable μ is the chemical potential.

Received by the editors August 15, 2017.
2000 *Mathematics Subject Classification.* 65M15, 35K25, 35K55.

We consider the initial condition $u(\mathbf{x},0) = u_0(\mathbf{x})$ and boundary conditions, i.e. $\mathbf{n}\cdot\nabla\mu = \mathbf{n}\cdot\nabla u = 0$, where $\mathbf{n}$ is the outward unit normal to $\partial\Omega$. $B(u) = 18u^2(1-u)^2$ is a double-well potential, $M(u) = 2B(u)$ a mobility function, $g(u) = 30u^2(1-u)^2$ an enhancing function, and ϵ relates to the thickness of the transition region between the two phases $u = 1$ and $u = 0$. The model formally converges for $\epsilon \to 0$ to Mullins sharp interface model for surface diffusion [35], see, in particular [42, 21, 56]. For the aformentioned result to hold the fourth order polynomial in u in the mobility function $M(u)$ is essential [56]. As recently shown [12, 31, 32] occasionally used second order polynomials in u in the mobility function $M(u)$, see e.g. [7, 58, 51, 27], do actually not converge to surface diffusion if $\epsilon \to 0$. Heuristic arguments and matched asymptotic analysis lead to the presence of an additional bulk diffusion term, which might alter the long time behavior. This is not the case for the originally proposed phase field approximation [9], which uses a double-obstacle potential instead of the double-well potential $B(u)$. The enhancing function $g(u)$ does not alter the matched asymptotic analysis. Such a function is commonly used in classical phase field models for solidification [29] to ensure better, though not necessarily higher convergence in ϵ. Herein we demonstrate its advantage to increasing the accuracy, especially for larger values of ϵ.

For $M(u) = g(u) = 1$ the classical Cahn-Hilliard equation [8] is recovered, which formally converges for $\epsilon \to 0$ to the Mullins-Sekerka problem [36], see [39]. The Cahn-Hilliard equation can be written in the abstract framework as the H^{-1} gradient flow $u_t = -\nabla_{H^{-1}}\mathcal{E}[u]$, with respect to the energy

$$\mathcal{E}(u) = \int_\Omega \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}B(u)\right)\, d\mathbf{x}. \tag{2}$$

Convexity splitting for the Cahn-Hilliard equation has been considered in e.g. [18, 6, 19]. In this work we start with the canonical nonlinear convex splitting $B(u) = B_c(u) - B_e(u)$, where

$$B_c(u) = B(u) + \alpha\left(u - \frac{1}{2}\right)^2, \qquad B_e(u) = \alpha\left(u - \frac{1}{2}\right)^2. \tag{3}$$

For $\alpha \geq 9$ the two function $B_c(u)$ and $B_e(u)$ are convex and thus also the energies $\mathcal{E}_c = \int_\Omega \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}B_c(u)\right) d\mathbf{x}$ and $\mathcal{E}_e = \int_\Omega \left(\frac{1}{\epsilon}B_e(u)\right) d\mathbf{x}$. The resulting convex splitting scheme is unconditionally energy stable, unconditionally solvable and converges optimally in the energy norm [19]. We will adapt this scheme and use it for eq. (1) with the above considered functional forms for $M(u)$ and $g(u)$. For $g(u) = 1$ the analytical results for the Cahn-Hilliard equation can be adapted to show energy stability properties also for the more general case [16]. But, if $g(u)$ in non-constant, we are unable to rigorously demonstrate the desired properties of the scheme, the model does not fall into the considered class of a gradient flow. It does not even have an energetic-variational structure. On the other side the improved accuracy of the model with $g(u)$ is absolutely essential to enable large scale simulations for surface diffusion, such as the complex solid-state dewetting scenarios of ultra-thin silicon films in [37]. For an introduction to solid-state dewetting see the review [50]. We therefore adapt the proposed scheme for the Cahn-Hilliard equation, consider a Rosenbrock time discretization to increase the accuracy of the scheme and apply it to the general case.

The paper is organized as follows: In Section 2 we describe the numerical approach in detail. We propose a first order scheme, for which we review unconditional energy stability for the case $g(u) = 1$. A modified linear first order scheme and a new Rosenbrock time stepping scheme is then introduced for the more general case.