Commun. Comput. Phys.
doi: 10.4208/cicp.scpde14.39s

Vol. **19**, No. 5, pp. 1473-1502
May 2016

On Fully Decoupled, Convergent Schemes for Diffuse Interface Models for Two-Phase Flow with General Mass Densities

Günther Grün[1,*], Francisco Guillén-González[2] and Stefan Metzger[1]

[1] *Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Cauerstr. 11, 91058 Erlangen, Germany.*
[2] *Universidad Sevilla, Dpto. Ecuaciones Diferenciales y Análisis Numérico, Instituto de Matemáticas, Aptdo. 1160, 41080, Sevilla, Spain.*

Received 6 March 2015; Accepted 7 December 2015

Abstract. In the first part, we study the convergence of discrete solutions to splitting schemes for two-phase flow with different mass densities suggested in [Guillen-Gonzalez, Tierra, J.Comput.Math. (6)2014]. They have been formulated for the diffuse interface model in [Abels, Garcke, Grün, M3AS, 2012, DOI:10.1142/S0218202511500138] which is consistent with thermodynamics. Our technique covers various discretization methods for phase-field energies, ranging from convex-concave splitting to difference quotient approaches for the double-well potential. In the second part of the paper, numerical experiments are presented in two space dimensions to identify discretizations of Cahn-Hilliard energies which are φ-stable and which do not reduce the acceleration of falling droplets. Finally, 3d simulations in axial symmetric geometries are shown to underline even more the full practicality of the approach.

AMS subject classifications: 35Q35, 65M60, 65M22, 65M12, 76D05, 76T10

Key words: Two-phase flow, Cahn-Hilliard equation, diffuse interface model, convergence of finite-element schemes, numerical simulation.

1 Introduction

In this paper, we are concerned with aspects of numerical analysis and practical computation related to the diffuse interface model for two-phase flow of incompressible, viscous

*Corresponding author. *Email addresses:* gruen@am.uni-erlangen.de (G. Grün), guillen@us.es (F. Guillén-González), stefan.metzger@fau.de (S. Metzger)

fluids with different mass densities proposed in [1]. It reads as follows.

$$\bar{\rho}(\varphi)\partial_t \mathbf{v} + \left(\left(\bar{\rho}(\varphi)\mathbf{v} + \frac{\partial\bar{\rho}(\varphi)}{\partial\varphi}\mathbf{j}\right)\cdot\nabla\right)\mathbf{v} - \nabla\cdot(2\eta(\varphi)\mathbf{D}\mathbf{v}) + \nabla p = \mu\nabla\varphi + \mathbf{k}_{\text{grav}}, \tag{1.1a}$$

$$\partial_t\varphi + \mathbf{v}\cdot\nabla\varphi - \nabla\cdot(M(\varphi)\nabla\mu) = 0, \tag{1.1b}$$

$$\mu = \sigma\big(-\varepsilon\Delta\varphi + \tfrac{1}{\varepsilon}F'(\varphi)\big), \tag{1.1c}$$

$$\nabla\cdot\mathbf{v} = 0 \quad \text{in } \Omega\times(0,T). \tag{1.1d}$$

Since we wish to take contact angle hysteresis into account, too, the following boundary conditions are chosen.

$$\sigma\frac{\partial\varphi}{\partial\mathbf{n}} = -\gamma_{LS}' - \alpha\partial_t\varphi \qquad \text{on } \partial\Omega\times(0,T), \tag{1.2a}$$

$$\frac{\partial}{\partial\mathbf{n}}\mu \equiv 0 \qquad \text{on } \partial\Omega\times(0,T), \tag{1.2b}$$

$$\mathbf{v} \equiv 0 \qquad \text{on } \partial\Omega\times(0,T). \tag{1.2c}$$

Here, $\gamma_{LS}(\phi)$ interpolates between the liquid-solid interfacial energies in the pure phases, and $\alpha \geq 0$ is the coefficient related to energy dissipation caused by contact line motion. The parameter σ is the surface tension coefficient, which is assumed to be $\sigma = 1$ in this paper. Note that this approach is inspired by the ideas of [22] where the relationship to contact angle hysteresis is explained. In particular, if $\gamma_{LS} \equiv const.$ and $\alpha \equiv 0$, the system prefers a contact angle θ of 90 degrees, as (1.2a) is a phase-field approximation of Young's law $\cos\theta = (\gamma_{LS}(-1) - \gamma_{LS}(1))/\sigma$, see [22]. Note that system (1.1) couples a hydrodynamic momentum equation with a Cahn-Hilliard type phase-field equation. F is a double-well potential with minima in ± 1 – representing the pure phases $\varphi \equiv \pm 1$. The term μ stands for the so called chemical potential, and the order parameter φ stands for the difference of the volume fractions $u_2 - u_1$ where $u_i(x,t) := \rho_i(x,t)/\tilde{\rho}_i$ with $\tilde{\rho}_i$ the specific (constant) density of fluid i in a unmixed setting. The parameter ε controls the width of the interface region. For the ease of notation we set $\varepsilon = 1$. Denoting the individual velocities by $\mathbf{v}_i$, $i = 1,2$, we write $\mathbf{v} := u_1\mathbf{v}_1 + u_2\mathbf{v}_2$ for the volume averaged velocity. Assuming $\tilde{\rho}_2 \geq \tilde{\rho}_1$, the density of the total mass $\bar{\rho}(\varphi)$ is given by

$$\bar{\rho}(\varphi) = \frac{\tilde{\rho}_2 + \tilde{\rho}_1}{2} + \frac{\tilde{\rho}_2 - \tilde{\rho}_1}{2}\varphi, \tag{1.3}$$

and $\mathbf{D}\mathbf{v}$ denotes the symmetrized gradient. The term $\mathbf{k}_{\text{grav}}$ stands for the density of external volume forces. Finally, the flux $\mathbf{j}$ is defined by $\mathbf{j} := -M(\varphi)\nabla\mu$ where $M(\varphi)$ is the mobility.

It is straightforward to show that the physical energy[†]

$$\overline{\mathcal{E}}(\mathbf{v},\varphi) := \frac{1}{2}\int_\Omega \bar{\rho}(\varphi)|\mathbf{v}|^2 + \frac{\varepsilon}{2}\int_\Omega |\nabla\varphi|^2 + \frac{1}{\varepsilon}\int_\Omega F(\varphi) + \int_{\partial\Omega}\gamma_{LS}(\varphi) \tag{1.4}$$

[†]Note that later in the paper, we will consider regularizations $\rho(\cdot)$ of $\bar{\rho}(\cdot)$. Consistently, we will denote the corresponding energy by $\mathcal{E}(\mathbf{v},\varphi)$.