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Unconditional Bound-Preserving and Energy-Dissipating Finite-Volume Schemes for the Cahn-Hilliard Equation

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Abstract. We propose finite-volume schemes for the Cahn-Hilliard equation which unconditionally and discretely preserve the boundedness of the phase field and the dissipation of the free energy. Our numerical framework is applicable to a variety of free-energy potentials, including Ginzburg-Landau and Flory-Huggins, to general wetting boundary conditions, and to degenerate mobilities. Its central thrust is the upwind methodology, which we combine with a semi-implicit formulation for the free-energy terms based on the classical convex-splitting approach. The extension of the schemes to an arbitrary number of dimensions is straightforward thanks to their dimensionally split nature, which allows to efficiently solve higher-dimensional problems with a simple parallelisation. The numerical schemes are validated and tested through a variety of examples, in different dimensions, and with various contact angles between droplets and substrates.

AMS subject classifications: 65M08, 35Q92, 35Q35, 35Q70

Key words: Cahn-Hilliard equation, diffuse interface theory, gradient flow, finite-volume method, bound preservation, energy dissipation.

1 Introduction

The Cahn-Hilliard (CH) equation is a popular phase-field model initially proposed in [18] to describe the process of phase separation in binary alloys. Since then, it has found innumerable applications, from capillarity–wetting phenomena [3,56] and diblock copolymer

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molecules [65] to tumour growth [39, 60], image inpainting [12, 16, 21] and topology optimization [66]; see the review [45].

Like all phase-field models, the CH equation avoids the explicit treatment of sharp interfaces altogether via thin transition regions through which pertinent variables and physical properties vary rapidly but continuously. It has a gradient-flow structure of the form

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left(M(\phi) \nabla \frac{\delta \mathcal{F}[\phi]}{\delta \phi} \right), \tag{1.1}$$

where ϕ is the *phase-field*, a continuous function of time and space which plays the role of an order parameter describing the phases of the system. In a binary system, the limiting values $\phi = 1$ and $\phi = -1$ represent each of the two phases. The *mobility* $M(\phi)$ may be *degenerate* [34, 44] with zeros at $\phi = \pm 1$,

$$M(\phi) = M_0(1-\phi)(1+\phi), \tag{1.2}$$

or may be taken as a constant, $M(\phi) = M_0$ [3].

The *free energy* $\mathcal{F}[\phi]$ of the solution to Eq. (1.1) is given by

$$\mathcal{F}[\phi] = \int_\Omega \left(H(\phi) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) \mathrm{d}\Omega + \int_{\partial\Omega} f_w(\phi, \beta) \, \mathrm{d}s, \tag{1.3}$$

where $H(\phi)$ is a double-well potential with minima at, or close to, $\phi = \pm 1$ which correspond to the stable phases in the system, ε is a positive parameter related to the width of the diffuse interface (see, for instance, [23]), and $f_w(\phi, \beta)$ is the wall free energy, a function of the phase field at the boundary parametrised by the equilibrium contact angle β [61]; see Fig. 1 for a schematic of a droplet on a solid substrate with contact angle β. The variation of the free energy with respect to the phase field, $\frac{\delta \mathcal{F}[\phi]}{\delta \phi}$, is known as the *chemical potential*, denoted ξ. The boundary conditions for (1.1) are a combination of the natural boundary condition for the wall free energy and the no-flux condition for the chemical potential [3, 47],

$$\varepsilon^2 \nabla \phi \cdot n = -f_w'(\phi, \beta), \quad M(\phi) \nabla \xi \cdot n = 0, \tag{1.4}$$

where n is an inward-pointing unit vector normal to the wall and $f_w'(\phi, \beta)$ denotes the derivative of $f_w(\phi, \beta)$ with respect to the phase-field.

The form of the term $f_w(\phi, \beta)$ has received considerable attention in the literature. Early contributions considered a linear form, see [52] for instance. Here we shall assume that the function f_w has bounded second derivative on $[-1, 1]$, so that it can be split into a convex part and a concave part satisfying

$$f_w(\phi, \beta) = f_{c,w}(\phi, \beta) - f_{e,w}(\phi, \beta), \tag{1.5}$$

where $f_{c,w}$ and $f_{e,w}$ are convex functions. A good choice is a cubic polynomial [3, 56–58]: the lowest-order polynomial which permits the minimization of the wall free energy for