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Two-phase flow with mass density contrast: Stable schemes for a thermodynamic consistent and frame-indifferent diffuse-interface model

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ABSTRACT

In this paper, we present a numerical scheme for the diffuse-interface model in [3] for two-phase flow of immiscible, incompressible fluids. As that model is in particular consistent with thermodynamics, energy estimates are expected to carry over to the discrete setting. By a subtle discretization of the convective coupling with the flux of the phase-field in the momentum equation, we prove discrete consistency with thermodynamics. Numerical experiments in two spatial dimensions – ranging from Rayleigh–Taylor instability to a comparison with previous modeling approaches – indicate the full practicality of our scheme and enable a first validation of the new modeling approach in [3].

1. Introduction

In [3], the following diffuse-interface model for two-phase flow of immiscible, incompressible fluids was introduced.

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

$$\operatorname{div}\mathbf{v} = 0, \tag{1.1b}$$

$$\partial_t\varphi + \mathbf{v}\cdot\nabla\varphi - \operatorname{div}\left(M(\varphi)\nabla\mu\right) = 0, \tag{1.1c}$$

$$\mu = \sigma\left(-\delta\Delta\varphi + \delta^{-1}F'(\varphi)\right) \quad \text{in } \Omega\times(0,T). \tag{1.1d}$$

As boundary conditions, no-slip conditions for $\mathbf{v}$ and the vanishing of the normal derivative of φ and of μ on $\partial\Omega\times(0,T)$ are imposed.

Note that system (1.1) constitutes a coupling of 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 $\varphi\equiv\pm1$. The parameter σ is the surface tension coefficient, which is assumed to be $\sigma=1$ if not stated explicitly. With a grain of salt, the positive parameter δ is a measure for the thickness of the diffuse-interface – for more details, see the discussion in the sequel about different approaches to model two-phase flows. The mobility $M(\varphi)$ is a non-negative function which can for instance be chosen constant or degenerate in ±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 $u_i(x,t) := \frac{\rho_i(x,t)}{\hat\rho_i}$ with $\hat\rho_i$ the specific (constant) density of fluid i in an unmixed setting. 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.

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The mass density $\rho(\varphi)$ is defined as

$$\rho(\varphi) = \frac{\hat{\rho}_2 + \hat{\rho}_1}{2} + \frac{\hat{\rho}_2 - \hat{\rho}_1}{2}\varphi$$

and $\mathbf{Dv}$ denotes the symmetrized gradient. The term $\mathbf{k}_{\text{grav}}$ stands for the density of external volume forces, within this article we only consider gravitational forces. Finally, the flux $\mathbf{j}$ is defined by $\mathbf{j} := -M(\varphi)\nabla\mu$.

System (1.1) may be derived from energy considerations and Onsager's variational principle. It is worth mentioning that material frame-indifference, i.e. the invariance of the system with respect to Galilean transformations, for instance, is sensitive to the question to which extent motions relatively to the barycentric motion are neglected in the momentum equation. In the predecessor paper [2], relative motions are totally neglected in the momentum equation. As a result, the system studied there turns out not to be frame-indifferent anymore. For more details on the derivation of the model studied here, we refer the reader to [3].

Conceptually, various approaches exist to model the flow of two immiscible, incompressible fluids. In sharp-interface models, the transition layer separating the two fluids is idealized to be a two-dimensional surface. In level-set methods, volume-of-fluids methods, and diffuse-interface models, additional order parameters are introduced which provide information whether fluid 1 or fluid 2 prevails in a spatial point x at time t.

In contrast to the former approaches, diffuse-interface models assume the transition layer to be of finite size. They are distinguished by the following features. No artificial additional conditions are necessary to model topology changes or to guarantee conservation of individual masses. Moreover, in many cases the convergence of discrete solutions to a solution of the underlying pde-system can be proven in a mathematically rigorous way. These advantages come at the prize of solving in addition a Cahn–Hilliard equation coupled to the momentum equation. Fortunately, adaptivity in space and time and a good analytical understanding of Cahn–Hilliard equations provide efficient strategies to keep the numerical cost very low compared to the cost of solving the momentum equation.

The idea of diffuse-interface models is to approximate the interfacial energy, which in the case of the sharp-interface model is proportional to the surface area of the interface, by the functional

$$A_\delta(\varphi) := \frac{\delta}{2}\int_\Omega |\nabla\varphi|^2 + \frac{1}{\delta}\int_\Omega F(\varphi) \tag{1.2}$$

where δ is a positive parameter which turns out to describe the width of the diffuse-interface (for a nice heuristic argument, see Chapter 6 of [7]). Modica and Mortola [22] and Modica [21] have shown that for $\delta \to 0$ the functional $A_\delta(\varphi)$ Γ-converges to the functional

$$A_0(\varphi) := \begin{cases} 2c_0 \int_\Omega |D\varphi| & \text{if } \varphi \in BV(\Omega) \text{ and } F(\varphi(x)) = 0 \text{ almost everywhere in } \Omega, \\ +\infty & \text{otherwise} \end{cases} \tag{1.3}$$

where $c_0 := \int_{-1}^{+1} \sqrt{F(s)}\, ds$.

Hence, A_0 is finite only for those functions in the space of functions of bounded variation ($BV(\Omega)$) which attain only values ± 1 except on a set of Lebesgue-measure zero. Note in particular that $\int_\Omega |D\varphi|$ is identical with the perimeter of the set $\{x \in \Omega \mid \varphi(x) = 1\}$.[1] Assuming this set to have a sufficiently smooth boundary, for instance a Lipschitz boundary, this perimeter is nothing else than the surface measure of the boundary. To put it in physical terms, it is nothing else than the area of the interface separating the different phases $\varphi = \pm 1$ (see [21] and the references therein). Hence, A_δ is an approximation of the surface area of the interface. This may serve as an explanation for the approximation property diffuse-interface models have with respect to sharp-interface models on the level of energies.

Another feature of diffuse-interface models is that often existence of solutions to the underlying system of partial differential equations can be proven global in time. This is desirable not only from the mathematical point of view. Such a result is available (or expected to be available) in the continuous setting as soon as the model is consistent with thermodynamics. In our context, this means that the energy at a time $t_2 > t_1$ is bounded by the sum of the energy at time t_1 and the work done by external forces during the time interval $[t_1, t_2]$. Especially in the framework of the system under consideration, we require that the sum of the kinetic energy $\frac{1}{2}\int_\Omega \rho|\mathbf{v}|^2$ and the interfacial energy $\int_\Omega \frac{\delta}{2}|\nabla\varphi|^2 + \delta^{-1}F(\varphi)$ is decreasing with respect to time when no external forces are considered.

Numerically, such a result is the key to prove stability and convergence results for appropriate schemes. In this sense, we introduce the *total energy* at time t as the sum of the discrete counterparts of the kinetic and the interfacial energy. We call a numerical scheme *stable* or *discretely consistent with thermodynamics* if the total energy at time $t_2 > t_1$ is bounded by the sum of the total energy at time t_1 and the work done by external forces during the time interval $[t_1, t_2]$.

Note that this notion of stability is in the spirit of *stability with respect to a norm*, see for instance [19, Definition 2.4.3].

Let us make a few more remarks on diffuse-interface models in general.

Historically, the first diffuse-interface model for two-phase flow was the so-called model H, introduced by Hohenberg and Halperin [17]. It assumed the mass densities of the two fluids to be identical.

[1] For more results on $BV(\Omega)$, we refer the reader to [11] and [29].