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A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow ☆

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ABSTRACT

A new time discretization scheme for the numerical simulation of two-phase flow governed by a thermodynamically consistent diffuse interface model is presented. The scheme is consistent in the sense that it allows for a discrete in time energy inequality. An adaptive spatial discretization is proposed that conserves the energy inequality in the fully discrete setting by applying a suitable post processing step to the adaptive cycle. For the fully discrete scheme a quasi-reliable error estimator is derived which estimates the error both of the flow velocity, and of the phase field. The validity of the energy inequality in the fully discrete setting is numerically investigated.

1. Introduction

In the present work we propose a stable and (essentially) linear time discretization scheme for two-phase flows governed by the diffuse interface model

$$\rho\partial_t v + ((\rho v + J)\cdot\nabla)\, v - \operatorname{div}(2\eta D v) + \nabla p = \mu\nabla\varphi + \rho g \qquad \forall x\in\Omega,\ \forall t\in I, \tag{1}$$

$$\operatorname{div}(v) = 0 \qquad \forall x\in\Omega,\ \forall t\in I, \tag{2}$$

$$\partial_t\varphi + v\cdot\nabla\varphi - \operatorname{div}(m\nabla\mu) = 0 \qquad \forall x\in\Omega,\ \forall t\in I, \tag{3}$$

$$-\sigma\epsilon\Delta\varphi + F'(\varphi) - \mu = 0 \qquad \forall x\in\Omega,\ \forall t\in I, \tag{4}$$

$$v(0,x) = v_0(x) \qquad \forall x\in\Omega, \tag{5}$$

$$\varphi(0,x) = \varphi_0(x) \qquad \forall x\in\Omega, \tag{6}$$

$$v(t,x) = 0 \qquad \forall x\in\partial\Omega,\ \forall t\in I, \tag{7}$$

$$\nabla\mu(t,x)\cdot\nu_\Omega = \nabla\varphi(t,x)\cdot\nu_\Omega = 0 \qquad \forall x\in\partial\Omega,\ \forall t\in I, \tag{8}$$

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where $J = -\frac{d\rho}{d\varphi} m\nabla\mu$. This model is proposed in [1]. Here $\Omega \subset \mathbb{R}^n$, $n \in \{2, 3\}$, denotes an open and bounded domain, $I = (0, T]$ with $0 < T < \infty$ a time interval, φ denotes the phase field, μ the chemical potential, v the volume averaged velocity, p the pressure, and $\rho = \rho(\varphi) = \frac{1}{2}((\rho_2 - \rho_1)\varphi + (\rho_1 + \rho_2))$ the mean density, where $0 < \rho_1 \le \rho_2$ denote the densities of the involved fluids. The viscosity is denoted by η and can be chosen arbitrarily, fulfilling $\eta(-1) = \tilde{\eta}_1$ and $\eta(1) = \tilde{\eta}_2$, with individual fluid viscosities η_1, η_2. The mobility is denoted by $m = m(\varphi)$. The gravitational force is denoted by g. By $Dv = \frac{1}{2}\left(\nabla v + (\nabla v)^t\right)$ we denote the symmetrized gradient. The scaled surface tension is denoted by σ and the interfacial width is proportional to ϵ. The free energy is denoted by F. For F we use a splitting $F = F_+ + F_-$, where F_+ is convex and F_- is concave.

The above model couples the Navier–Stokes equations (1)–(2) to the Cahn–Hilliard model (3)–(4) in a thermodynamically consistent way, i.e. a free energy inequality holds. It is the main goal to introduce and analyze an (essentially) linear time discretization scheme for the numerical treatment of (1)–(8), which also on the discrete level fulfills the free energy inequality. This in conclusion leads to a stable scheme that is thermodynamically consistent on the discrete level.

Existence of weak solutions to system (1)–(8) for a specific class of free energies F is shown in [2,3]. See also the work [27], where the existence of weak solutions for a different class of free energies F is shown by passing to the limit in a numerical scheme. We refer to [6,13,22,37], and the review [8] for other diffuse interface models for two-phase incompressible flow. Numerical approaches for different variants of the Navier–Stokes Cahn–Hilliard system have been studied in [7,13,25,27–29,32], and [36].

This work is organized as follows. In Section 3 we derive a weak formulation of (1)–(8) and in Section 5 formulate a time discretization scheme. In Section 6 we derive the fully discrete model and show the existence of solutions for both the time discrete, and the fully discrete model, as well as energy inequalities, both for the time discrete model, and for the fully discrete model. In Section 7 we use the energy inequality to derive a residual based adaptive concept, and in Section 8 we numerically investigate properties of our simulation scheme.

2. Notation

Let $\Omega \subset \mathbb{R}^n$, $n \in \{2, 3\}$ denote a bounded domain with boundary $\partial\Omega$ and outer normal ν_Ω. Let $I = (0, T]$ denote a time interval.

We use the conventional notation for Sobolev and Hilbert Spaces, see e.g. [4]. With $L^p(\Omega)$, $1 \le p \le \infty$, we denote the space of measurable functions on Ω, whose modulus to the power p is Lebesgue-integrable. $L^\infty(\Omega)$ denotes the space of measurable functions on Ω, which are essentially bounded. For $p = 2$ we denote by $L^2(\Omega)$ the space of square integrable functions on Ω with inner product $(\cdot, \cdot)$ and norm $\|\cdot\|$. For a subset $D \subset \Omega$ and functions $f, g \in L^2(\Omega)$ we by $(f, g)_D$ denote the inner product of f and g restricted to D, and by $\|f\|_D$ the respective norm. By $W^{k,p}(\Omega)$, $k \ge 1, 1 \le p \le \infty$, we denote the Sobolev space of functions admitting weak derivatives up to order k in $L^p(\Omega)$. If $p = 2$ we write $H^k(\Omega)$. The subset $H^1_0(\Omega)$ denotes $H^1(\Omega)$ functions with vanishing boundary trace.

We further set

$$L^2_{(0)}(\Omega) = \{v \in L^2(\Omega) \,|\, (v, 1) = 0\},$$

and with

$$H(\mathrm{div}, \Omega) = \{v \in H^1_0(\Omega)^n \,|\, (\mathrm{div}(v), q) = 0 \,\forall q \in L^2_{(0)}(\Omega)\}$$

we denote the space of all weakly solenoidal $H^1_0(\Omega)$ vector fields.

For $u \in L^q(\Omega)^n$, $q > n$, and $v, w \in H^1(\Omega)^n$ we introduce the trilinear form

$$a(u, v, w) = \frac{1}{2}\int_\Omega ((u \cdot \nabla)\, v)\, w \, dx - \frac{1}{2}\int_\Omega ((u \cdot \nabla)\, w)\, v \, dx. \tag{9}$$

Note that there holds $a(u, v, w) = -a(u, w, v)$, and especially $a(u, v, v) = 0$.

3. Weak formulation

In the present section we formulate a weak formulation of (1)–(8). To begin with, note that for a sufficiently smooth solution (φ, μ, v) of (1)–(8) and using the linearity of ρ it holds

$$\partial_t \rho + \mathrm{div}\,(\rho v + J) = 0,$$

see [1, p. 14]. Using this mass balance we can rewrite (1) as

$$\partial_t(\rho v) + \mathrm{div}\,(\rho v \otimes v) + \mathrm{div}\,(v \otimes J) - \mathrm{div}\,(2\eta Dv) + \nabla p = \mu\nabla\varphi + \rho g. \tag{10}$$

We also note that the term $\rho v + J$ in (1) is not solenoidal (which might lead to difficulties both in the analytical and the numerical treatment) and that the trilinear form $(((\rho v + J) \cdot \nabla)u, w)$ is not anti-symmetric. To obtain a weak formulation yielding an anti-symmetric convection term we use a convex combination of (1) and (10) to define a weak formulation. We multiply equations (1) and (10) by the solenoidal test function $\frac{1}{2}w \in H(\mathrm{div}, \Omega)$, integrate over Ω, add the resulting equations and perform integration by parts. This gives