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An adaptive finite element Moreau–Yosida-based solver for a coupled Cahn–Hilliard/Navier–Stokes system

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ABSTRACT

An adaptive a posteriori error estimator based finite element method for the numerical solution of a coupled Cahn–Hilliard/Navier–Stokes system with a double-obstacle homogenous free (interfacial) energy density is proposed. A semi-implicit Euler scheme for the time-integration is applied which results in a system coupling a quasi-Stokes or Oseen-type problem for the fluid flow to a variational inequality for the concentration and the chemical potential according to the Cahn–Hilliard model [16]. A Moreau–Yosida regularization is employed which relaxes the constraints contained in the variational inequality and, thus, enables semi-smooth Newton solvers with locally superlinear convergence in function space. Moreover, upon discretization this yields a mesh independent method for a fixed relaxation parameter. For the finite dimensional approximation of the concentration and the chemical potential piecewise linear and globally continuous finite elements are used, and for the numerical approximation of the fluid velocity Taylor–Hood finite elements are employed. The paper ends by a report on numerical examples showing the efficiency of the new method.

1. Introduction

In the present work we consider a diffuse interface model for the description of the hydrodynamics of two-phase flows, which is related to model ‘H’ in the nomenclature of Hohenberg and Halperin [35]. It can be found, e.g., in [1] and reads:

Find $(c(t,x), w(t,x), \mathbf{u}(t,x), p(t,x))$ such that

$$\partial_t \mathbf{u} - \frac{1}{Re}\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p + Kc\nabla w = 0 \quad \text{in } \Omega_T := \Omega\times(0,T), \tag{1.1}$$

$$\operatorname{div}\mathbf{u} = 0 \quad \text{in } \Omega_T, \tag{1.2}$$

$$\partial_t c - \frac{1}{Pe}\nabla\cdot(b(c)\nabla w) + \mathbf{u}\nabla c = 0 \quad \text{in } \Omega_T, \tag{1.3}$$

$$w = \Phi'(c) - \gamma^2\Delta c \quad \text{in } \Omega_T, \tag{1.4}$$

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$$c(x,0) = c^0(x), \quad \mathbf{u}(x,0) = \mathbf{u}^0(x) \ \forall x \in \Omega, \tag{1.5}$$

$$\partial_\nu c = \partial_\nu w = 0, \quad \mathbf{u} = \mathbf{g} \quad \text{on } \partial\Omega \times (0,T). \tag{1.6}$$

Here $\Omega \subset \mathbb{R}^n,\ n \in \{1,2,3\}$, is the bounded convex polygonal flow domain with boundary $\partial\Omega$ and outer unit normal ν. We note that more general domains with sufficiently smooth boundary may be used as well. The function

$$c = \frac{c_A - c_B}{c_A + c_B},$$

defined on Ω_T, denotes the concentration order parameter associated with the mass concentrations c_A and c_B in the fluid phases A and B, respectively. It satisfies $c = c(t,x) \in [-1,1]$ and $c \equiv 1$ in the pure A-phase and $c \equiv -1$ in the pure B-phase region, respectively. Initially, i.e. for $t = 0$, we assume that the concentration equals c^0. The quantity w represents the chemical potential, $\mathbf{u}$ denotes the mean flow velocity field, i.e. $\mathbf{u} = \frac{1+c}{2}\mathbf{u}_A + \frac{1-c}{2}\mathbf{u}_B$, where $\mathbf{u}_A$ and $\mathbf{u}_B$ are the fluid velocities in the fluid phases A and B, respectively, and p denotes the pressure of the fluid. The flow profile at $t = 0$ is given by $\mathbf{u}^0$. The boundary values $\mathbf{g}$ have to satisfy $\mathbf{g} \cdot \nu = 0$ and are assumed to satisfy $\mathbf{g} \equiv 0$ in the following. The Péclet number Pe, the Reynolds number Re and the capillary number K are given constants. The given parameter γ is related to the width of the interface region. The mobility function $b(\cdot)$ is assumed to be equal to 1 but other situations can be motivated by practical applications and are considered for example in [3].

The homogeneous free energy density is denoted by $\Phi(c)$ and in this paper it is chosen to be of double-obstacle type as proposed in [6] (see also [19]), i.e.

$$\Phi(c) := \begin{cases} \frac{1}{2}(1 - c^2) & \text{if } c \in [-1,1], \\ +\infty & \text{if } c \notin [-1,1]. \end{cases}$$

In the literature, alternative choices of the homogeneous free energy density are known with the double-well [22] and the logarithmic potential [16] being two common alternatives. Note that in contrast to the double-obstacle potential, the double-well potential allows the unphysical situation of $|c| > 1$. The logarithmic potential, on the other hand, usually prevents reaching the pure phases due to the barrier nature of the involved logarithm. When $\Phi(c)$ is chosen to be the double-obstacle potential, then (1.4) becomes

$$w + \gamma^2 \Delta c \in \partial\Phi(c) \tag{1.7}$$

where $\partial\Phi$ is the subdifferential of Φ. Let us recall that the subdifferential $\partial I_{\{|c| \leqslant 1\}}(v)$ of the indicator functional

$$I_{\{|c|\leqslant 1\}}(v) := \begin{cases} 0, & |\, v \,| \leqslant 1, \\ \infty, & \text{else}, \end{cases}$$

defined on $H^1(\Omega)$ for $|\, v \,| \leqslant 1$ a.e. in Ω consists of all functionals $\xi \in H^1(\Omega)^*$, the dual space of $H^1(\Omega)$, satisfying $\langle \xi, z - v \rangle \leqslant 0$ for all $z \in H^1(\Omega), |\, z \,| \leqslant 1$ a.e. in Ω. It then follows from subdifferential calculus (see e.g. [24]) that the potential Eq. (1.7) is equivalent to

$$|c| \leqslant 1 \text{ a.e. in } \Omega, \left\langle -\gamma^2 \Delta c - w - c, v - c \right\rangle \geqslant 0 \quad \forall v \ \in \{v \in H^1(\Omega) | |v| \leqslant 1 \quad \text{a.e. in } \Omega\}. \tag{1.8}$$

Here and below, 'a.e. in Ω' stands for 'almost everywhere in Ω' indicating that the associated relation holds true except on a subset of Ω which has (Lebesgue-) measure zero.

In what follows, $L^2(\Omega)$ denotes the space of measurable functions whose square is Lebesgue integrable with inner product $(\cdot,\cdot)$ and norm $\|\cdot\|$. By $L^2_{(0)}(\Omega) \subset L^2(\Omega)$ we denote the subspace of functions with vanishing mean value and $H^m(\Omega),\ m \geqslant 1$, represents the usual Hilbert space of functions in $L^2(\Omega)$ with distributional derivatives of order less or equal m contained in $L^2(\Omega)$. The norm in $H^m(\Omega)$ is denoted by $\|\cdot\|_m$. We define $H^1_0(\Omega)$ by

$$H^1_0(\Omega) = \{v \in H^1(\Omega) | v = 0 \text{ on } \partial\Omega\},$$

where the boundary condition holds true in the sense of traces. Let $\mathbf{H}^m(\Omega) = (H^m(\Omega))^n$ and analogously for $H^m_0(\Omega)$. The dual spaces of $H^1_0(\Omega)$ and $\mathbf{H}^1_0(\Omega)$ are denoted by $H^{-1}(\Omega)$ and $\mathbf{H}^{-1}(\Omega)$, respectively. For $D \subset \Omega$ we denote by $(\cdot,\cdot)_{m,D}, \|\cdot\|_{m,D}$ and $|\cdot|_{m,D}$ the usual inner-product, the norm and the semi-norm in $H^m(D)$, respectively.

Furthermore we set

$$\mathcal{V} = \{v \in H^1(\Omega) | (v, 1) = 0\}$$

and

$$\mathcal{K} = \{v \in H^1(\Omega) | |v| \leqslant 1 \text{ a.e. in } \Omega\}.$$

For more information on Lebesgue and Sobolov spaces we refer the reader to [2].

Based on the above definitions and conventions, the variational form of (1.1)–(1.6) reads:

Find $(c(t), w(t), \mathbf{u}(t), p(t))$ in $\mathcal{K} \times H^1(\Omega) \times \mathbf{H}^1_0(\Omega) \times L^2_{(0)}(\Omega)$ such that