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A HYBRID LEVEL–SET–CAHN–HILLIARD MODEL FOR TWO-PHASE FLOW

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ABSTRACT

We present a hybrid level–set–Cahn–Hilliard model for the simulation of two phase flow in micro structures. Our method combines accurate contact line dynamics in the Cahn–Hilliard equation with the computationally cheaper level set method in regions where not the full Cahn–Hilliard dynamics are necessary to describe the flow. This is realized by employing the Cahn–Hilliard model close to rigid boundaries, together with a level set method away from boundaries. We use a level set formulation with smoothed color function so that the interface representation in both regions is the same. The combined model is coupled to the incompressible Navier–Stokes equations, where the surface tension acts as a forcing term, calculated by the stress form in the Cahn–Hilliard model and a continuous surface tension representation for the level set part. A continuous function is used as a switch between the two models, retaining mass conservation of the overall method. The gains of the method are twofold — the equations to be solved in the interior are structurally easier than the Cahn–Hilliard equation and, more importantly, the level set model can accurately model two-phase flow already at coarser meshes. For oil expulsion by inflowing water we are able to obtain results of comparable quality when using less elements than with a Cahn–Hilliard model on the whole domain.

1. INTRODUCTION

The phase field model, based on the coupled Cahn–Hilliard–Navier–Stokes equations, is a phenomenological model for the simulation of the dynamics of two-phase flow [6], [11], [2]. The basic concept of the phase field model is the representation of two fluid phases by two minima of a double-well potential with a smooth transition region representing the interface. The form and width of the transition region between the two phases gives rise to surface tension forces that enter the Navier–Stokes equations, cf. [11]. In the phase field model, there are two transport mechanisms that move fluid–fluid interfaces. The first one is the advective transport of the interface by the fluid velocity while the second one is diffusive mass transport. It is very challenging to numerically solve the coupled Cahn–Hilliard–Navier–Stokes system. Structural difficulties are the non-linearity of the Cahn–Hilliard equation, the presence of fourth order partial derivatives, and, in addition, the coupling to the Navier–Stokes equations, a set of equations that already in itself is expensive to treat. Moreover, the transition region between the two fluids is typically chosen to be very narrow, which implies a rapid change of the concentration order parameter, whereby steep gradients occur. It is of key importance to sufficiently resolve the interface region in space since the information in the gradients governs the surface tension force. High resolution in time is required as well because of a wide range of time scales in the Cahn–Hilliard model. Even though considerable progress has been made in recent years regarding the efficient numerical simulation of the phase field model (such as locally refined grids and nonlinear multigrid routines [12]), the performance

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of phase-field based simulation strategies is still rather unsatisfactory. Most of the applications of the model in the literature (see, e.g., references in [12], [15]) are therefore limited to micro scale calculations.

An established approach for macro scale multiphase flow simulations is the level set method [14]. The basic concept of level set approaches is to define the interface implicitly as a (zero) level set of a function, the level set function. The traditional choice for the level set function has been a signed distance function, where the function modulus describes the distance to the fluid-fluid interface and the sign distinguishes the fluids. The motion of the interface is achieved by advection of the level set function with local fluid speed. However, in such a model it is not straightforward to define consistent surface tension forces that enter the Navier–Stokes equations [7]. In recent years, progress has been made in directly applying level set functions that mimic smoothed color (indicator) functions, by making use of suited numerical methods that retain steep gradients and conserve mass [13]. The advantage of this kind of models is the possibility to directly apply a continuum definition of surface tension [3], such that no indirect force reconstruction is needed. The overall advantage of level set models, its ease of use, has the price that contact lines at rigid boundaries are difficult to move correctly. Level set implementations require a sufficient resolution of the interface as well, which can be accounted for by adaptive mesh refinement. Though, the resolution demands in level set models are less severe compared to Cahn–Hilliard models.

The contribution of this work is to combine the phase field method and the level set method to form a hybrid method, designed for simulations at length scales larger than the ones usually employed in phase field based models, while still including correct contact line dynamics. The basis of our considerations is the similar shape of the concentration function in the Cahn–Hilliard model and the smoothed color function in the level set model. Also the definition of surface tension forces shows close similarities between the models. Though, the transport mechanisms are more sophisticated for the Cahn–Hilliard equation. For this initiatory study, we consider flows where the convective mass transport dominates the diffusive mass transport, making the two models resemble each other even closer. Nevertheless, we keep the different properties of the two models, so that overall consistency is retained. We account for this difference by a continuous filtering function that acts as a switch between the models. Close to the boundary, we employ a Cahn–Hilliard model that enables the motion of contact lines at walls with fluid-specific contact angles. In the interior, we switch to the computationally more efficient level set model and thereby avoid to resolve the full nonlinear structure in the Cahn–Hilliard equation. The construction principle of our hybrid method is inspired by approaches used for simulating turbulent flows, where a Reynolds–averaged Navier–Stokes (RANS) method close to boundaries and large eddy simulations (LES) in the interior have successfully been coupled to form a promising hybrid method [8].

The outline of this article is as follows. In section 2, we present the constituents to our hybrid model, the Cahn–Hilliard and the level set model, which we then combine to a hybrid model. Section 3 discusses the numerical implementation of the model within a finite element environment including adaptive grid refinement. Section 4 presents a numerical example using the new method, and section 5 finally gives conclusions and indicates further research directions.

2. DEVELOPING THE HYBRID MODEL

We develop a hybrid level–set–Cahn–Hilliard model that is applicable to two-phase flow involving fluids of different densities, viscosities, includes the effect of surface tension, allows for external forces such as gravity and is able to correctly represent moving contact lines. We base the notation on the classical Cahn–Hilliard notation as used in [2], which we use even for the level set part of the model in the same form.

2.1 Flow equations

The zero level set of a color function $c \in [-1, 1]$ is used to describe the interface. In fluid 1, $c(\mathbf{x}) \approx 1$, and in fluid 2, $c(\mathbf{x}) \approx -1$. In the Cahn–Hilliard equation the color function is a measure of the concentration order parameter, while in the level set region it is a smoothed indicator function. We denote by ρ_1^0 and ρ_2^0 the densities and by μ_1^0 and μ_2^0 the dynamic viscosities of fluids 1 and 2, respectively. Since we want to formulate our model

in non-dimensionalized form, we define dimensionless parameters

$$\rho = 1 + \frac{\rho^\delta}{2}(c-1), \qquad \mu = \frac{1}{\mathrm{Re}}\left(1 + \frac{\mu^\delta}{2}(c-1)\right) \tag{1}$$

that represent the density and viscosity in the two phase model. The variables $\rho^\delta = (\rho_1^0 - \rho_2^0)/\rho_1^0$ and $\mu^\delta = (\mu_1^0 - \mu_2^0)/\mu_1^0$ denote the differences in the material parameters of density and viscosity (assuming that the density of fluid 1 is larger than of fluid 2), and $\mathrm{Re} = \rho_1^0 U_c L_c/\mu_1^0$ denotes the Reynolds number of the flow, involving the characteristic length scale L_c and the characteristic velocity scale U_c [15]. In this work, we consider laminar flow at small Reynolds number. The governing equations of fluid motion are the incompressible Navier–Stokes equations in the velocity $\mathbf{u}$ and the pressure p,

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \nabla(2\mu\,\varepsilon(\mathbf{u})) + \nabla p = \rho\mathbf{e}_g + \mathbf{f}_{\mathrm{st}}, \qquad \nabla\cdot\mathbf{u} = 0, \tag{2}$$

where $\varepsilon(\mathbf{u}) = \left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)/2$ denotes the rate of deformation tensor and $\mathbf{f}_{\mathrm{st}}$ the force due to surface tension, which will be specified by the models in the subsequent sections. The vector $\mathbf{e}_g$ denotes the direction of gravity. The Navier–Stokes equations have to hold within the computational domain Ω in d-dimensional space for all simulation times $t \in (0, T]$. The Navier–Stokes equations are completed by a divergence–free initial velocity field and boundary conditions specified by the application problem.

2.2 Cahn–Hilliard model

The convective Cahn–Hilliard equation describes the motion of a function c under the velocity field $\mathbf{u}$ and is given by

$$\begin{aligned} \frac{\partial c}{\partial t} + \nabla\cdot(\mathbf{u}c) - \frac{1}{\mathrm{Pe}}\nabla\cdot\left(\frac{b(c)}{\rho}\nabla w\right) &= 0, \\ -\rho w + \frac{1}{\epsilon}\Phi'(c) - \epsilon\Delta c &= 0, \end{aligned} \tag{3}$$

where the Péclet number Pe specifies the amount of diffusive mass transport in the Cahn–Hilliard equation, the mobility function is $b(c) = (\max(1-c^2, 0))^2$, w represents a modified chemical potential, ϵ is a measure of the interface width of the order $\mathcal{O}(\epsilon)$, and $\Phi(c) = (1-c^2)^2/4$ denotes the double well potential. The operator $'$ denotes the derivative with respect to c. The function c is a concentration measure — the fraction of fluid 1 of the total volume is given by $(1+c)/2$ and the fraction of fluid 2 is $(1-c)/2$. The second equation in (3) is the equation of the chemical potential and balances the double well potential with the diffusion in c. The smaller ϵ is, the narrower the interface will be represented in the model. For computational convenience, we have chosen to define a modified chemical potential w by $w = \widetilde{w}\rho$ based on the true Cahn–Hilliard potential $\widetilde{w}$ as used in [2], [11]. The Cahn–Hilliard equation was orginally proposed as one equation in c only [4], but in order for the numerical discretization with H^1 conforming finite elements [5] to be applicable, we use the mixed form, see section 3.1. Note that system (3) conserves mass [12].

The Cahn–Hilliard equation is a space-time dependent system to hold in $\Omega \times (0, T]$ and needs to be closed by appropriate boundary conditions. Following the reasoning in [15], we want to be able to prescribe oblique static contact angles to the chemical potential. The conditions for achieving this are

$$\mathbf{n}\cdot\nabla w = 0, \qquad \mathbf{n}\cdot\nabla c = -k g'(c), \tag{4}$$

where $\mathbf{n}$ denotes the unit outer normal on the domain boundary $\partial\Omega$, k is the so-called wetting coefficient and $g(c) = c(3-c^2)/4$ denotes a local surface energy, see [11] and [15] for details. The wetting parameter k controls the static contact angle θ_e at wall boundaries through $k = \cos(\theta_e)$.

The force $\mathbf{f}_{\mathrm{st}}$ due to surface tension in the phase field model, here in stress form [12], is defined by

$$\mathbf{f}_{\mathrm{st}} = \frac{\rho}{\mathrm{Ca}} w\nabla c + \frac{\rho^\delta}{\mathrm{Ca}}\frac{1-c^2}{4}\nabla w, \tag{5}$$

where the capillary number $\mathrm{Ca} = 2\sqrt{2}\mu_1^0 U_c/3\sigma$ defines the ratio between viscous and tension forces, specified through the equilibrium surface tension σ of a plane interface, cf. [15].

2.3 Conservative level set model

The level set formulation we are going to use closely resembles the method developed in [13], where a smoothed color function is used as the level set function. This interpretation has the advantage that the concentration variable c in the Cahn–Hilliard model is nothing else but a special smoothed color function [11]. Starting from an initial profile c, the motion of the color level set function obeys a basic convection equation,

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = 0. \tag{6}$$

It is well-known, though, that any plain numerical method for advancing this profile in time will eventually distort the profile, either by oscillations or smearing. This already happens for the conventional level set formulations with a signed distance function (having well-behaved gradients), and is even more important for the color function where the profile rapidly switches from -1 to 1. For example, transition regions of a moving droplet will be advanced differently at upwind and downwind sides, respectively. In order to prevent such undesired behavior, a problem-adapted stabilization technique has been developed [13]. The idea is to employ stabilization that can restore the profile shape without (substantially) moving the interface. Since we use a formulation of c in $[-1, 1]$ compared to the interval $[0, 1]$ used in [13], we select the modified stabilization procedure

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{n}(1 - c^2) - \nabla \cdot \mathbf{n}(\eta \nabla \cdot \mathbf{n}c) = 0, \tag{7}$$

where the normal $\mathbf{n} = \nabla c/|\nabla c|$ points perpendicular to the gradient and $\eta = \mathcal{O}(h)$ is a diffusion parameter of the order of the mesh size h that brings in diffusion in normal direction. The compressive flux, the second term in (7), is constructed in a way that information from regions with $c < 0$ will be transported towards the interface. In practice, this means that a value of -1 is transported towards the interface until it is compensated by the normal diffusion. The same mechanism is acting in regions where $c > 0$. The steady state of (7) is a regular profile as desired. This procedure also provides a suitable initial field when only interface points are specified. The stabilization (7) is mass-conservative [13].

The force due to surface tension, finally, is given by the diffuse interface approach introduced in [3], which can be directly applied in this context, yielding

$$\mathbf{f}_{\mathrm{st}} = \frac{2}{\mathrm{We}} \kappa \nabla c, \tag{8}$$

where $\mathrm{We} = \rho U_c^2 L_c/\rho$ is the non-dimensional Weber number measuring the surface tension force, and the curvature of the interface is $\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot (\nabla c/|\nabla c|)$. The factor 2 in (8) accounts for the different definition of c as compared to [3].

2.4 Combination of the two models

As been emphasized by the common notation in sections 2.2 and 2.3, there is a close relation between the Cahn–Hilliard equation and the above level set method with continuum surface tension force. It was already pointed out in [11] that the interface representation in the phase field model actually is a continuum surface tension model with appropriate scaling. Since we want to be able to exploit the similarities irrespective such a scaling, we follow an equation coupling technique as used in [8] to account for the different terms in the two models (3) and (6). We start by defining a function $\alpha(\mathbf{x})$ that is constant 1 close to rigid boundaries and constant 0 far away from them. In the transition region, we let $\alpha(\mathbf{x}) = r((x_i - s_1)/s_2)$, where the function $r(y) = y^2(y-2)^2$ implements a continuous switch from 0 to 1 in the interval $[0, 1]$, s_1 denotes the starting position of the switch in coordinate direction i, and s_2 is the width of the transition region. See figure 1 for a schematic one-dimensional representation of the function $\alpha(x)$. With this at hand, let

$$\mathcal{M} = \alpha(\mathbf{x})\mathcal{M}_1 + (1 - \alpha(\mathbf{x}))\mathcal{M}_2, \tag{9}$$

with $\mathcal{M}_{1/2}$ representing Cahn–Hilliard and level set model, respectively, and $\mathcal{M}$ their combination.

The filtering framework (10) will now be applied to combine system (3) with the system formed by (6) together with the equation for the curvature, $\kappa = -\nabla \cdot (\nabla c/|\nabla c|)$, to give one model for the dynamics of the

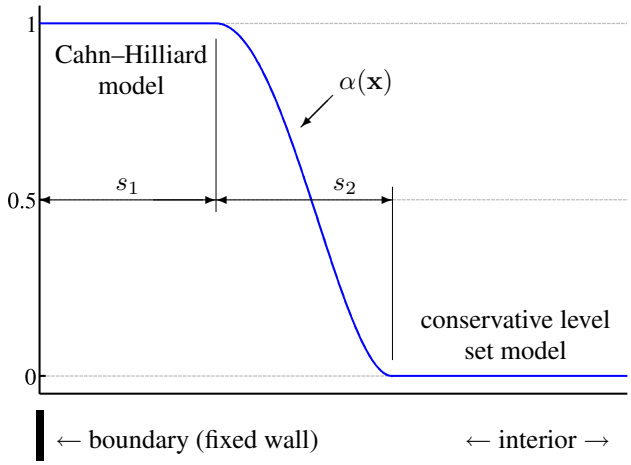

Figure 1: Schematic illustration of the switch function $\alpha(\mathbf{x})$ in one dimension.

interface. We use the pair of variables (c, w) to denote the concentration and chemical potential in the Cahn–Hilliard region and the concentration and curvature times density in the level set region. We shall call w pseudo potential in the following. The hybrid model for the interface advection reads

$$\begin{aligned} \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) - \frac{1}{\mathrm{Pe}} \nabla \cdot \left(\alpha \frac{b(c)}{\rho} \nabla w \right) = 0, \\ -\rho w + \frac{\alpha}{\epsilon} \Phi'(c) - \epsilon \nabla \cdot (\alpha \nabla c) - \nabla \cdot \left((1-\alpha) \frac{\nabla c}{|\nabla c|} \right) = 0. \end{aligned} \tag{10}$$

We can use the boundary conditions (4) for this combined system because the Cahn–Hilliard model is applied in boundary regions and needs therefore to be fed with boundary data. System (10) needs to hold on the domain Ω for all times t. The definition of the surface tension force according to the model (9) is

$$\mathbf{f}_{\mathrm{st}} = \alpha \left(\frac{\rho}{\mathrm{Ca}} w \nabla c + \frac{\rho^\delta}{\mathrm{Ca}} \frac{1-c^2}{4} \nabla w \right) + (1-\alpha) \left(\frac{1}{\mathrm{We}} w \nabla c \right). \tag{11}$$

The density in the definition of the level set force has been absorbed into the compound variable w.

3. NUMERICAL IMPLEMENTATION

Multiphase flow situations generally occur in rather complicated geometries. Moreover, the use of adaptive meshes should be possible. Hence, we base our implementation of the hybrid method derived in section on the framework of finite elements.

3.1 Discretization

We need to solve the coupled system of the Navier–Stokes equation (2) and the hybrid level–set–Cahn–Hilliard system (10). This is a system of nonlinear partial differential equations in d-dimensional space and time, totaling in $d + 3$ coupled equations. The time derivatives in $\mathbf{u}$ and c are discretized using a BDF-2 time integration scheme (backward differentiation formula [9]), that is a numerical method suited for stiff equations as the ones at hand. The method is fully implicit, so we have to perform a nonlinear iteration. During this iteration, we solve the Navier–Stokes equations first with c and w from the previous iteration inserted into (11), which updates $\mathbf{u}$ and p, see section 3.1.1. The updated velocity will then be used for the solution of system (10), see section 3.1.2. This process is started for some prediction $(\mathbf{u}_0^n, p_0^n, c_0^n, w_0^n)$, where n denotes the time step and the subscript 0 the iteration index. The prediction is obtained by extrapolation using the time stepping scheme. The solution process represents a nonlinear Gauss–Seidel iteration in the 2×2 block system of $(\mathbf{u}, p)$ and (c, w), respectively.

3.1.1 Navier–Stokes equations

We choose to solve the Navier–Stokes equations in a coupled way, i.e., we solve for velocity and pressure simultaneously at each step of the nonlinear iteration. Compared to decoupled solution methods, this strategy allows for larger time steps without having any numerical inbalances between pressure and velocity, at the price of considerably higher workload per step. For the discretization in space, we use a finite element discretization. For the saddle-point structure of the Navier–Stokes system, the interpolation spaces for velocity and pressure need to satisfy a stability condition in order to constitute a stable discrete system, the so-called inf–sup (LBB) condition, cf. [5]. To fulfill this condition, we choose the inf–sup stable Taylor–Hood element pair, i.e., quadratic basis functions for the velocity and linear basis functions for the pressure. The nonlinear convective term is accounted for by a Picard iteration. The resulting time-discretized and linearized finite element formulation of the Navier–Stokes system reads:
Find $(\mathbf{u}_i^n, p_i^n)$ at time level n and nonlinear iteration i, such that

$$\begin{aligned}\left(\boldsymbol{\phi}_k, \rho_{i-1}\frac{3\mathbf{u}_i^n}{2\Delta t}\right)_\Omega + \left(\boldsymbol{\phi}_k, \rho_{i-1}\mathbf{u}_{i-1}^n\cdot\nabla\mathbf{u}_i^n\right)_\Omega + \left(\nabla\boldsymbol{\phi}_k, 2\mu_{i-1}\varepsilon(\mathbf{u}_i^n)\right)_\Omega - \left(\nabla\boldsymbol{\phi}_k, p_i^n\right)_\Omega \\ + \left(\psi_l, \nabla\cdot\mathbf{u}_i^n\right)_\Omega = \left(\boldsymbol{\phi}_k, \rho_{i-1}\left(\frac{2\mathbf{u}^{n-1}}{\Delta t} - \frac{\mathbf{u}^{n-2}}{2\Delta t}\right)\right)_\Omega + \left(\boldsymbol{\phi}_k, \rho_{i-1}\mathbf{e}_g + \mathbf{f}_{\mathrm{st},i-1}\right)_\Omega\end{aligned} \tag{12}$$

holds for all finite element basis functions $(\boldsymbol{\phi}_k, \psi_l)$ in the respective finite-dimensional test function spaces. As indicated by the index $i-1$, the surface tension force is evaluated with values (c_{i-1}, w_{i-1}) according to (11). The same linearization is applied to density and viscosity using relation (1). The term Δt denotes the time step size and $(\cdot,\cdot)_\Omega$ is the standard L_2 inner product on Ω. The solution functions for velocity and pressure are linear combinations of the finite element basis functions

$$\mathbf{u}_i^n = \sum_k \boldsymbol{\phi}_k u_k, \qquad p_i^n = \sum_l \psi_l p_l, \tag{13}$$

where the parameters u_k, p_l are nodal degrees of freedom. Some of them may be fixed by boundary conditions.

3.1.2 Level–Set–Cahn–Hilliard system

We use the updated velocity for calculating (c_i^n, w_i^n) by the level–set–Cahn–Hilliard model (10) and use a fixed point iteration to linearize the nonlinear bulk energy and the normal to c. The nonlinear parameters in the diffusive term of the concentration equation are evaluated at the previous iteration. The spatial part is discretized using linear finite elements for both the concentration and the pseudo potential. Since the first equation of system (10) is a convection-dominated equation, a straight-forward finite element discretization of the equation would introduce spurious oscillations around the steep gradient of c [5]. In order to avoid this, we stabilize the equation with a streamline upwind Petrov–Galerkin (SUPG) approach [5]. The SUPG stabilization method introduces an additional term $(\mathbf{u}_i^n\cdot\nabla\chi_k, \tau_{\mathrm{stab}} r(c_i^n))_\Omega$ with the residual $r(c_i^n) = 3c_i^n/(2\Delta t) - \mathbf{u}_i^n\cdot c_i^n - 2c^{n-1} - c^{n-2}$ and stabilization parameter $\tau_{\mathrm{stab}} = \mathcal{O}(h)$ as given in [5]. Note that r is the *true* residual also for the Cahn–Hilliard region, since the second derivative of the linear basis functions is zero. Moreover, the calculation of curvature in the level set region is stabilized by an extra diffusion term $-(1-\alpha)h\nabla^2 w$ for an element size of h according to [13], which avoids oscillations in w. The resulting (time-discretized and linearized) system is:
Find (c_i^n, w_i^n) at time level n and nonlinear iteration i, such that

$$\begin{aligned}\left(\chi_k, \frac{3c_i^n}{2\Delta t}\right)_\Omega - \left(\mathbf{u}\cdot\nabla\chi_k, c_i^n - \tau_{\mathrm{stab}} r(c_i^n)\right)_\Omega + \left(\nabla\chi_k, \frac{\alpha b(c_{i-1}^n)}{\mathrm{Pe}\rho_{i-1}}\nabla w_i^n\right)_\Omega - \left(\vartheta_l, \rho_{i-1} w_i^n\right)_\Omega \\ + \left(\nabla\vartheta_l, \alpha\epsilon\nabla c_i^n\right)_\Omega = \left(\chi_k, \left(\frac{2c^{n-1}}{\Delta t} - \frac{c^{n-2}}{2\Delta t}\right)\right)_\Omega - \left(\vartheta_l, \frac{\alpha}{\epsilon}\Phi'(c_{i-1}^n)\right)_\Omega \\ - \left(\nabla\vartheta_l, \frac{(1-\alpha)\nabla c_{i-1}^n}{|\nabla c_{i-1}^n|}\right)_\Omega - \left(\vartheta_l, k g'(c_{i-1}^n)\right)_{\partial\Omega,\mathrm{wall}}\end{aligned} \tag{14}$$

for all finite element test functions (χ_k, ϑ_l). The finite element approximations c_i^n and w_i^n are, as in (13), given by a linear combination of linear basis functions.

3.1.3 Reinitialization

The level set part of the domain is still subject to the problems discussed in section 2.3, i.e., distortion of the profile. Therefore, we perform a reinitialization procedure according to (7) in the level set part each fifth time step. This procedure means finding a steady state. Since the numerical distortion of the profile can be expected to be little after a few steps only, the steady state of (7) is usually reached in two to three time steps. In order to prevent spurious oscillations close to the interface, we combine the procedure with a step of a diffusive equation in the beginning of the reinitialization. Since we close this equation with Neumann boundary conditions, the masses in both fluids remain unchanged. In order to give the level set interface region a similar shape as the Cahn–Hilliard part, we choose the diffusion parameter $\eta = \max(3\epsilon/2, h)$, where the additional h aims at keeping the reinitialization procedure free from oscillations.

3.1.4 Spurious currents

The continuum surface approach used in our model is subject to spurious velocity currents in situations where capillary effects dominate (e.g. in situations without external sources), an effect that is caused by numerical imbalances between the surface tension force $\mathbf{f}_{\mathrm{st}}$ and the pressure gradient, as explained e.g. in [10]. So far, we have not made any additional attempt to prevent this situation in our model, but we plan to do so in the future.

3.1.5 Code details

We implemented systems (12) and (14) in deal.II, an open source C++ finite element library collection, based on quadrilateral elements [1]. The equations are used to construct large sparse linear equation systems, which, for the time being, are solved with an ILU preconditioned GMRES method (Navier–Stokes) and with a direct solve (level–set–Cahn–Hilliard system), respectively. The computational costs for this procedure are moderate. For example, a mesh with 8,192 finite elements in 2D results in 66,306 degrees of freedom for velocity and 8,385 degrees of freedom for pressure, concentration and pseudo potential, respectively. On a 2.4 GHz AMD Opteron system, one time step consisting of three nonlinear iterations of such a system is executed in 15–20 seconds when running the program in serial (single-threaded). Most of the time is spent for the solution of linear systems, so additional benefits can be expected by the use of better linear algebra routines, which we intend to do in the future, such as the algorithm presented in [12].

3.2 Adaptive mesh refinement

As mentioned in the introduction, an efficient realization of the above equations relies in an accurate resolution of the interface. In the Cahn–Hilliard region, more than 98 percent of the surface tension is induced in the region $c \in [-0.9, 0.9]$ [11], which implies that an accurate representation of the interface is necessary. On the other hand, the dynamics in the rest of the domain are usually rather uninteresting. Therefore, we implement an adaptive mesh strategy in order to better resolve the interface region without increasing the numerical costs too much. Based on the concentration function c, we construct the error indicator

$$\gamma(\mathbf{x}) = \frac{1}{\epsilon}(1 - c^2(\mathbf{x})), \tag{15}$$

which reaches its maximum at $c = 0$ and is almost zero in regions far away from the interface. We calculate the L_2 norm of γ on each cell. If $\|\gamma\|_{\mathrm{cell}} \geq 0.7$, we mask a cell for refinement in the next step. On the contrary, we coarsen regions where all child cells satisfy $\|\gamma\|_{\mathrm{cell}} \leq 0.35$. The definition of the cell-wise L_2 norm already accounts for different element lengths.

We complete our adaptivity implementation by a complementary control of the maximum refinement level. Since the curvature in the level set model is less sensitive than the Cahn–Hilliard potential, we can reduce the highest refinement level by one in the level set region, without any considerable effect on the surface tension. Since we do not want to reset the mesh in every time step, we let the finest resolved region consist of about 20 elements so that it is possible to perform up to 20 time steps without remeshing. Besides that, we do not let the mesh get too coarse far away from the interface in order to maintain a certain accuracy in the Navier–Stokes solution there as well. The hanging nodes, occurring for the adaptively refined structured meshes we use, are eliminated by deal.II library functions, ensuring consistency of the mesh refinement [1].

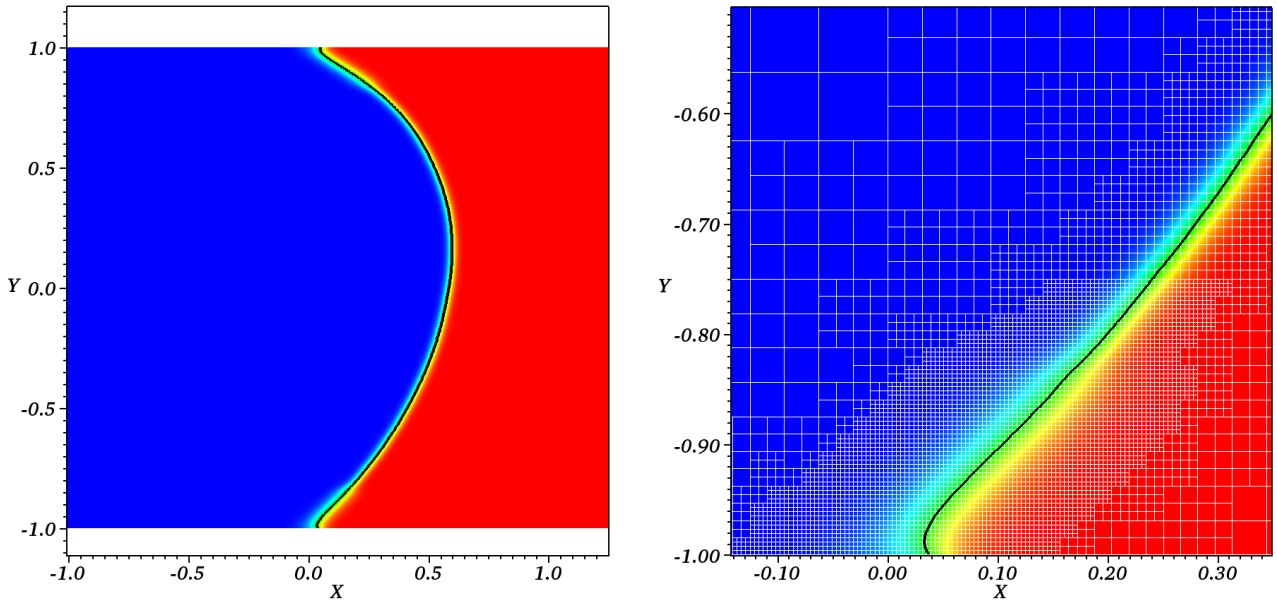

Figure 2: Results with the hybrid model at $t = 1$, including the adaptive grid structure close to the lower boundary (right). To the left, the whole interface is shown. The black line shows the interface position (zero level set), the blue and red color represent the two fluid phases. Note the finer mesh in the Cahn–Hilliard region close to the boundary.

4. COMPUTATIONAL EXAMPLE

We test our method on a two phase flow problem in a channel. We perform the calculations in dimensionless units, with channel dimensions $[-2, 2] \times [-1, 1]$. We assume fixed walls in y-direction with zero Dirichlet (no-slip) conditions on the velocity in the Navier–Stokes system and open boundaries at $x = \pm 2$. We consider parameters that are typical for water and oil for flows at length scales of a few millimeters with a Reynolds number $\mathrm{Re} = 1$, $\rho^\delta = 0.27$, $\mu^\delta = -0.0023$, and we neglect the effects of gravity. In the level–set–Cahn–Hilliard system, we choose $\mathrm{Pe} = 100$, $\mathrm{Ca} = 20$, $\mathrm{Fr} = 200$, set the interface thickness $\epsilon = 0.01$ and use a contact angle of 40 degrees between the wall and the interface, measured from the water side ($k = 0.77$). We choose $s_1 = 0.85$, $s_2 = 0.1$ as parameters for the level–set–Cahn–Hilliard switch, meaning that the Cahn–Hilliard region is 0.15 units thick, and the transition occurs in another 0.1 units, compare also Fig. 1. The element size of the discretization ranges from 0.06 units to 0.004 units, see Fig. 2 for a representation of the adaptive mesh structure. The time step is chosen to be 0.0066. We stop the nonlinear iteration as soon as the error is reduced by a factor of 10^3, which is usually achieved after two to three nonlinear iterations.

The example represents an inflow-driven oil expulsion from the channel. As a boundary condition, we prescribe a quadratic inflow data on the left. On the right end of the channel, zero Neumann data is applied on the Navier–Stokes system. We start from a zero velocity profile at $t = 0$ with the interface located at $x = 0$ and a contact line at the static contact angle. The inflow velocity is then successively increased, with the peak velocity at the channel center obeying $u_1 = \sin(\pi t/2)$ until $t = 1$ is reached. Then, we keep the velocity at a value of 1. Figs. 2 and 3 show results for this configuration at $t = 1$ and $t = 1.4$. In the two pictures, the number of elements is 16,500 and 20,000, respectively. In comparison to a Cahn–Hilliard model on the whole domain (employing about 30,000 elements), our model shows accurate results. Even the prediction of the contact line motion at the lower boundary is quite accurate — it deviates by about 4% from the high resolved Cahn–Hilliard equation. The results for this problem show an asymmetry in the interface position with respect to the channel center, an effect that we want to study further in the future.

5. CONCLUSIONS

A hybrid method that combines the advantageous features of level set methods and the phase field model has been presented. The method is implemented using a finite element method and is shown to give good results

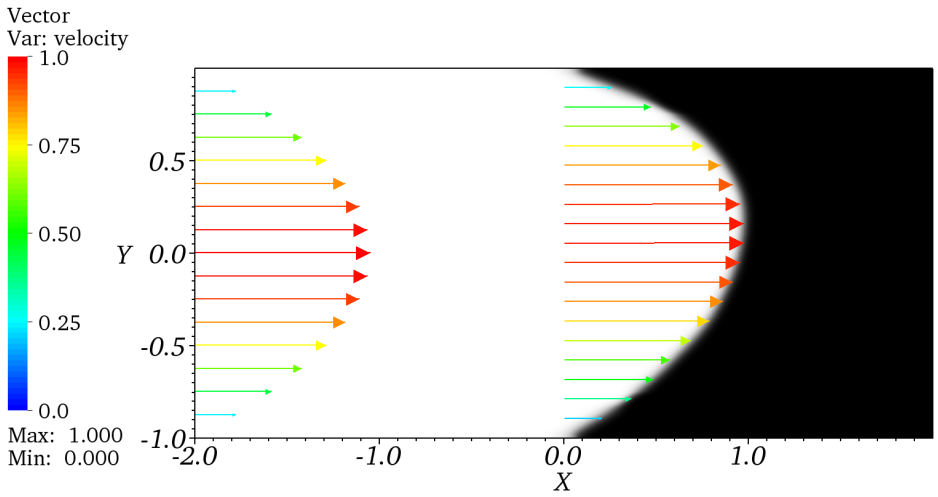

Figure 3: Interface position and some velocity values at $t = 1.4$. To the left, the inflow is depicted. The velocity close to the interface shows a similar profile, but is slightly unsymmetric (with respect to the channel center) at this stage of the simulation.

for the simulation of two-phase flow in a channel. Using the information of the phase field method close to boundaries, we have been able to reproduce correct contact line dynamics (as for the phase field model), combined with the ease of a level set approach in the interior where only surface tension forces are active. A numerical study on a inflow-driven channel flow shows good results. Considerable savings of the method can be achieved by solving simpler equations and by using coarser grids. However, we observed some minor deviations in the contact angle for the hybrid method compared to the full Cahn–Hilliard model, which we have to analyze quantitatively in the future.

We intend to continue the development of this method and to test it on other examples like contact-line driven flows as well as other material combinations besides the water–oil example considered in this report. Regarding the algorithm's efficiency, we want to improve the solution of the arising linear equation systems for both the Navier–Stokes system and the hybrid level–set–Cahn–Hilliard system. Moreover, we plan to use projection schemes for cheaper Navier–Stokes solutions of large 3D problems and to improve the adaptive mesh control, possibly by using different grids for the Navier–Stokes part and the interface representation part. We aim also at including the reinitialization procedure for the level set formulation directly in the model, which makes the global model more compact.

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