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Contact line treatment with the sharp interface method

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ABSTRACT

A technique to handle contact points in a sharp interface method based on the level set method is presented. The contact points are tracked explicitly. The coupling between the contact points and the zero level set is enforced by boundary conditions during reinitialisation of the distance function. For sharp interface methods an accurate approximation of the curvature is important. However, this cannot be obtained by using the conventional central difference methods adjacent to walls since the level set functions are not defined therein. Therefore we propose to use the tracked contact point and the intersection points of the first two grid lines parallel to the wall with the zero contour line of the signed distance function to approximate the contact angle and curvature adjacent to the walls. The method is verified using a capillary rise and a gravity driven two phase channel flow.

1. Introduction

Multi phase flows with moving contact lines can be found in many industrial and natural processes. Applications where the dynamics around the contact line plays an important role include microfluidics, coating processes, ink-jet printing or simple raindrops on the windscreen of a car.

Moving contact lines are a challenging problem to model. If the conventional no-slip boundary condition is applied to the Navier–Stokes equations, the stresses are diverging at the line where the three phases meet. In fact, molecular dynamics (MD) simulations show a nearly complete slip in the region of the contact line [1]. Over the years the moving contact line has been an topic of research and a lot of different theories have been developed to describe its dynamics [2,3].

Methods to model multi phase flows on fixed grids can be divided into two groups depending on the interface thickness. The first group assumes that the interface between the fluids is much smaller than any resolved length scale. Typically the interface is advected with the local fluid velocity and a number of different techniques exist to keep track of the interface position. These include the level set method [4] the volume of fluid method [5] and interface tracking methods [6]. On the other hand phase field methods solve the coupled Cahn–Hilliard/Navier–Stokes equations. The Cahn–Hilliard equation is based on the free energy of an interface [7] and therefore the interface extends over a finite region. The phase field methods allow for contact line movement through diffusive interfacial fluxes across the interface, even if a no-slip boundary condition is applied, which is not the case for methods which do not resolve the interface. The advantage of methods not resolving the interface is, that they typically require less resolution since the diffuse interface does not need to be resolved by a certain number of grid points.

An additional challenge for the first group has been that conventional discretisations can neither handle fluid properties which change instantly at the interface nor the singular surface tension force. The majority of methods for the modelling of multi phase flows including contact lines [8–11] smear out the jumps of the fluid properties over several grid points and the surface tension is implemented using the continuous surface force [12] or a similar method where the singular force is distributed over several grid points adjacent to the interface. The ghost-fluid method (GFM) [13] was extended to incompressible two phase flows [14] and it modifies the discretisation stencils to allow sharp jumps of the fluid properties at the interface as well as a sharp implementation of the surface tension force through a jump in the pressure.

The aim of the present study is to present a technique, which allows to handle contact lines in the context of a sharp interface method using the GFM. Moreover the method should be general in a way that it gives control over the contact point position. This is opposed to the more common approach manioulating the contact angle [8,9,18]. The presented method is a refinement of the technique presented in [15] and was used to implement a multi scale method for capillary driven multi phase flows [16,26]. The current paper focuses on the details of the numerical implementation of the contact point tracking and it is organised as follows. In Chapter 2 the governing equations for incompressible tow phase

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flow are introduced. The discretisation of the equations by the GFM and the implementation of the contact point tracking are described in Chapter 3. In chapter 4 the method is assessed for capillary rise and a moving contact point in a channel. Conclusions are stated in Chapter 5.

2. Equations

2.1. Navier–Stokes equations

We consider incompressible flow of two immiscible viscous fluids. In this study we confine ourselves to two-dimensional problems. The continuity and momentum equations, i.e., the Navier–Stokes equations for a Newtonian fluid for incompressible flow:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} + \rho\mathbf{g} \tag{2}$$

where $\mathbf{u}$ is the velocity vector, p is the pressure, $\mathbf{g}$ is the gravity vector, μ and ρ are the dynamic viscosity and the density, respectively. The material properties μ and ρ can be different in each fluid and we use a + and − sign to discriminate between the two fluids. These equations have to be fulfilled in both fluids in two phase flow.

2.2. Interface conditions

The boundary conditions at the interface can be derived by considering an infinitesimal control volume across the interface. This volume can be divided into a control volume for each fluid. The conservation laws for mass and momentum hold for the entire volume as well as for each of the partial volumes. Subtracting the sum of the conservation laws applied to the two partial volumes individually from the conservation laws applied to the entire volume, we get the boundary conditions at the interface. For the case with constant surface tension σ and no mass transfer across the interface the following jump conditions are obtained:

$$[\mathbf{u}] = 0 \tag{3}$$

$$\left[\begin{pmatrix}\mathbf{n}^T\\ \mathbf{t}^T\end{pmatrix}(p\mathbf{I}-\boldsymbol{\tau})\mathbf{n}\right] = \begin{pmatrix}\sigma\kappa\\ 0\end{pmatrix} \tag{4}$$

where square brackets define the jump across the interface, e.g. $[\mathbf{u}] = \mathbf{u}^+ - \mathbf{u}^-$. We further denote $\mathbf{n}$ and $\mathbf{t}$ as unit normal and tangent vectors to the interface. κ is the local interface curvature and τ is the viscous stress tensor. These conditions imply that the velocity and tangential stresses are continuous across the interface, whereas the pressure and the normal stresses are discontinuous.

2.3. Level set method

In order to apply the interface conditions presented in the previous section it is necessary to know its position. A popular method to keep track of the interface position in two phase flows is the level set method (LSM) [4], in which the interface is defined as the zero contour line of a scalar function ϕ. Typically ϕ is the signed distance function from the interface. It exists and is continuous in the entire computation domain. The signed distance function is advected with the local fluid velocity using the advection equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = 0 \tag{5}$$

Since all discretisations of the advection equation will not be exact, ϕ looses its signed distance property over time and has to be reinitialised solving the following equation to steady state

$$\frac{\partial \phi}{\partial \tau} + \mathrm{sign}(\phi)(|\nabla\phi| - 1) = 0 \tag{6}$$

The interface normal and curvature can be obtained directly from the signed distance function.

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{7}$$

$$\kappa = -\nabla\cdot\mathbf{n} \tag{8}$$

2.4. Contact point

Around a point where the interface between two fluids meets a solid surface, the conventional no-slip boundary condition cannot be applied. For otherwise the stresses around the interface would become singular. To avoid this singularity the no-slip boundary condition is often replaced by a slip boundary condition of the following form:

$$u_\parallel = \lambda\left.\frac{\partial u_\parallel}{\partial x_\perp}\right|_{\mathrm{wall}} \tag{9}$$

where λ is the slip length and $\parallel$ and $\perp$ denote the parallel and normal directions relative to the wall. The difference in the surface energies can lead to a motion of the contact point. For small capillary numbers this effect can become extremely important. However, it is not possible to describe the dynamics around the contact point accurately using the Navier–Stokes equations. Some authors choose to fix the contact angle to model the dynamics around the contact line [17,9,18]. In the present paper we shall set the contact point velocity u_{CP} as a function of the contact angle. To achieve this goal Spelt [10] proposed to track the contact point explicitly. Thus, the position of the contact point is described by an ordinary differential equation

$$\frac{\mathrm{d}x_{\mathrm{CP}}}{\mathrm{d}t} = u_{\mathrm{CP}} = f(\theta_{\mathrm{CP}}) \tag{10}$$

where $f(\theta_{\mathrm{CP}})$ is a function describing the dependency of the contact point velocity on the contact angle. The choice of f is important and should be done carefully to obtain reliable results. Different approaches to model the dependency of the contact point velocity on the contact angle are possible, including the use of empirical data or results from microscale simulations around the interface. The method presented here is not restricted to contact point velocities which are a function of the contact angle. In principle $f(\theta)$ can be replaced by any relation.

3. Discretisation

The discretisation is done on a uniform staggered grid, where the scalar quantities, i.e., pressure p and signed distance function ϕ, are stored at the cell centres while the velocity components u and v are stored at the vertical and horizontal cell faces, respectively [19]. The classical marker and cell (MAC) method is used to couple velocity and pressure in the discretisation of the incompressible Navier–Stokes Eqs. (1) and (2).

3.1. Navier–Stokes

The advection terms in the Navier–Stokes Eq. (2) are discretised by a 5th order Hamilton–Jacobi WENO scheme [13]. For the WENO scheme can handle the discontinuities in the first derivative of the velocity automatically. In points which are not adjacent to the interface the viscous terms are discretised by second order central difference stencils, i.e.,