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Reinitialization of the Level-Set Function in 3d Simulation of Moving Contact Lines

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Abstract. The level set method is one of the most successful methods for the simulation of multi-phase flows. To keep the level set function close the signed distance function, the level set function is constantly reinitialized by solving a Hamilton-Jacobi type of equation during the simulation. When the fluid interface intersects with a solid wall, a moving contact line forms and the reinitialization of the level set function requires a boundary condition in certain regions on the wall. In this work, we propose to use the dynamic contact angle, which is extended from the contact line, as the boundary condition for the reinitialization of the level set function. The reinitialization equation and the equation for the normal extension of the dynamic contact angle form a coupled system and are solved simultaneously. The extension equation is solved on the wall and it provides the boundary condition for the reinitialization equation; the level set function provides the directions along which the contact angle is extended from the contact line. The coupled system is solved using the 3rd order TVD Runge-Kutta method and the Godunov scheme. The Godunov scheme automatically identifies the regions where the angle condition needs to be imposed. The numerical method is illustrated by examples in three dimensions.

AMS subject classifications: 65Z05, 76T10

Key words: Level set method, two-phase flows, moving contact lines, contact angle, reinitialization, level set function.

1 Introduction

Contact line refers to the line where a fluid interface intersects with a solid wall. The modeling and simulation of moving contact lines have attracted much attention in recent years. This is not only due to the many industrial applications, e.g. in microfluidics, but

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also scientific interests such as the stress singularity, contact angle hysteresis, etc.. We refer to the review articles [1–4] and the monographs [5–7] for discussions of the current status of the moving contact lines problem.

Some numerical methods have been developed for the simulation of multi-phase flows with moving contact lines. These include the volume of fluids method [8–10], the front tracking method [11, 12], the phase field method [13–16], the level set method [17–20], etc.. More can be found in a recent review paper [21]. In this paper, we will focus on the level set method, in particular, the boundary condition for the reinitialization of the level set function in the simulation of the moving contact lines in three dimensions (3d).

In the level set method, the interface is implicitly represented using the zero-level set of a function $\phi(\mathbf{x})$, which is called the level set function. Usually the signed distance function is used as the level set function. It is evolved according to the velocity field of the fluids $\mathbf{u}$,

$$\frac{\partial \phi}{\partial t}+\mathbf{u}\cdot\nabla\phi=0. \tag{1.1}$$

During the evolution, the level set function is usually distorted in the sense that it deviates from the signed distance function and develops large variations. This may affect the accuracy of the numerical solution. To prevent this from happening, the level set function is reinitialized during the evolution. This is done by solving the following reinitialization equation in pseudo time τ [22]:

$$\frac{\partial \phi}{\partial \tau}+S(\phi_0)\left(|\nabla\phi|-1\right)=0, \tag{1.2}$$

where ϕ_0 is the level set function before the reinitialization, and $S(\cdot)$ is the sign function. Eq. (1.2) is a transport equation with the velocity

$$\mathbf{v}_\phi=S(\phi_0)\mathbf{n}, \quad \text{where} \quad \mathbf{n}=\frac{\nabla\phi}{|\nabla\phi|}. \tag{1.3}$$

Denote the outward unit normal of the wall by $\mathbf{n}_w$, then it is readily seen that Eq. (1.2) needs a boundary condition in regions where $\mathbf{v}_\phi\cdot\mathbf{n}_w<0$ (i.e. when the transport velocity points into the fluid domain) on the wall; in contrast, no boundary condition can be imposed in regions where $\mathbf{v}_\phi\cdot\mathbf{n}_w>0$. This is illustrated in Fig. 1, where the fluid interface is indicated by the bold curve. To reinitialize the given level set function shown in the figure, a boundary condition is needed on the wall outside the droplet, whereas no boundary condition is needed inside the droplet. After solving the reinitialization equation, the level set function becomes the signed distance function to the interface, except in the wedge (shaded region) where the level set function depends on the boundary condition specified on the wall.

Several strategies have been proposed regarding the boundary condition for the reinitialization equation. Most of these methods are for 2d problems as shown in Fig. 1, in