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Level set reinitialization at a contact line

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A B S T R A C T

When a level-set signed distance function is reinitialized in the vicinity of a contact line, there is a "blind spot" that prevents an accurate reconstruction of a signed distance function. The numerical method can create parasitic velocity currents near this region. If additional contact-line physics are included, the parasitic velocity currents would pollute the solution and alter the physical behavior. In this study, a modified reinitialization routine is proposed that combines the standard Hamilton–Jacobi equation with a relaxation equation for those grid cells along a wall in the blind spot. Two test cases, an angled fluid wedge (zero curvature) and a circular fluid arc (constant curvature), are used to evaluate the numerical error induced by different methods. The proposed method has less numerically-induced interface distortion than other techniques examined. Furthermore, this routine can be easily extended to three dimensions. Drops sliding on a wall are simulated in both two and three dimensions to demonstrate the advantages of this method. A spreading fluid interface further shows that this method allows contact lines to merge naturally.

1. Introduction

Whenever two fluids meet on a solid wall, a contact line is formed between the three phases. Contact lines are ubiquitous in many industrial and practical applications such as gas and oil recovery in porous media, inkjet printing, and droplet shearing from aerodynamic structures [1–4]. While there are many different computational techniques to simulate these problems [5–8], the level-set method is often preferred for its natural handling of topological changes and simple, accurate methods for interface curvature calculation [9]. Accurate calculation of the curvature is especially important for fluid flows with small capillary (Ca) and Weber (We) numbers. Under these conditions, surface tension σ dominates viscous and inertial effects; thus even small numerical curvature errors can incorrectly distort fluid interfaces from the physical solution. This paper examines the difficulties inherent in using a signed-distance-function level set in the vicinity of a contact line and proposes a new technique with small numerical curvature errors and subsequent interface deformations.

In the level set method, the fluid interface is embedded as the zero value of a scalar variable ϕ [10]. The choice of ϕ is arbitrary, but it is subject to two constraints: it must be smooth and continuous. These constraints allow accurate interpolation of the zero level set and computation of isocontour normal vectors $\vec{n}$ and curvatures κ,

$$\vec{n} = \frac{\nabla\phi}{|\nabla\phi|}, \qquad \kappa = -\nabla\cdot\phi. \tag{1}$$

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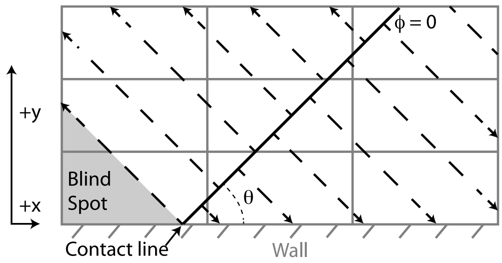

Fig. 1. Diagram of the blind spot (grey). The black solid line corresponds to the interface $\phi = 0$. The dashed lines are the characteristics for the Hamilton–Jacobi equation which are perpendicular to the interface.

Two common choices of ϕ are a signed distance function (interface $\phi = 0$) [11,12] and a conservative hyperbolic tangent distance function [13–15] (interface $\phi = 0.5$). While these methods differ in implementation, they both suffer the same problem in the vicinity of a contact line. While the solution implementations would differ, the concepts are the same. The signed distance function only is considered in this study.

The levelset function ϕ is typically evolved in two steps: a convection step and a reinitialization step. First, to transport the interface, the level-set variable ϕ is advected with the fluid velocity $\vec{u}$ to determine the new interface location using an advection transport equation

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0. \tag{2}$$

Unfortunately, after transport, ϕ is in general no longer a distance function. While the simulation can proceed using a non-distance function ϕ, the constraints (namely, smooth and continuous) may no longer be satisfied after multiple iterations. The reinitialization step attempts to return ϕ to a signed distance function ($|\nabla \phi| = 1$) while conserving the location of the zero level set and thus the fluid volume. A standard reinitialization technique integrates the Hamilton–Jacobi equation given by

$$\frac{\partial \phi}{\partial \tau} + \mathrm{sign}(\phi_0)\big(|\nabla \phi| - 1\big) = 0 \tag{3}$$

in pseudo-time τ [5]. ϕ_0 is the value of ϕ prior to reinitialization. This equation is hyperbolic and its characteristics are normal to the interface $\phi = 0$ (Fig. 1). While the reinitialization works well if no contact lines are present, a "blind spot" occurs with contact lines: there is a region where no characteristics exist because any characteristic would originate at the wall. This region will always occur on the obtuse-angle side of the interface, and it vanishes only if the angle at the wall is $\theta = 90°$ (hereafter this wall portion is referred to as the obtuse side). The mathematical solution for the Hamilton–Jacobi equation is, therefore, not well-posed because it lacks the proper boundary conditions. The resulting blind spot causes poor calculations of interface curvature at the contact line and creates parasitic currents. Over time, these currents cause spurious interface evolution.

To remedy this interface deformation, most previous studies have enforced a contact angle in the blind spot in one of two ways. In some cases, the blind spot contours have a pre-specified contact angle θ [14,16–18]. This contact angle (spatially uniform and constant in time) is usually chosen as the static contact angle. In other cases, a dynamic contact-angle law is used to impose a different angle value θ_D at each time step [2,19–21]. This contact angle is only spatially uniform in the vicinity of a contact line.

Forcing the angle in these ways has three problems. First, *a priori* knowledge of a dynamic contact angle law is required and, thus, the angle does not arise from physical mechanisms in the simulation. If there were a consensus on a dynamic contact angle law, using such a relation would represent the missing physics and would provide a basis for reinitialization. However, as discussed by Blake [22], there are numerous theories at this time and their applicability varies. Further, Yokoi et al. [2] showed a strong dependence of droplet spreading on the applied contact-angle law. They found the correct spreading radius in time only when the contact angle was prescribed by an experimentally-observed relation. Second, using either method, the isocontours have the same contact angle near the contact line. For a surface of constant curvature, such as a circular droplet, the isocontours have a spatially varying contact angle at the wall. This aspect is not captured by either technique. Lastly, imposing a contact angle moves the zero level set from its previous position. As a consequence, conservation of mass is often violated locally by the reinitialization procedure. More importantly, this forced angle distorts the interface and, in particular, the curvature distortion leads to parasitic currents.

There are three alternative method classes to mitigate the curvature errors caused by reinitialization in the blind spot. The first class uses more complex level-set transport schemes to preserve the quality of the interface curvature and remove the need for reinitialization [23–25]. These schemes often still require boundary conditions on the wall for the level set and, thus, may have a similar problem in the blind spot. The second class decouples the curvature at the wall from the level set curvature. In a recent work, Sato and Ničeno [26] used this approach with the curvature methods outlined by Brackbill et al. in [27]. In another study, Deganello et al. applied a curvature at the wall not calculated from the level set, but was derived