Numerical simulations of dynamic wetting

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Overview

Recently, there has been significant research directed at modeling of interfacial flows with “**contact lines**" (the lines that form where a fluid/fluid interface meets a solid surface) numerically, experimentally, and analytically. Due to rich fundamental hydrodynamics, the motion of a fluid in the proximity of a moving contact line is a very complex process.

$$\cos\theta_e = \frac{\gamma_{sg} - \gamma_{s\ell}}{\gamma_{\ell g}}$$

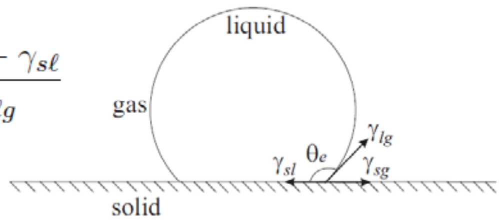

Figure 1: A solid-liquid-gas contact line at equilibrium.

Numerical modeling of Contact Lines

A three-dimensional numerical model to predict flows with dynamic contact lines is developed. The model presents a robust and accurate approach for contact line-driven flows. The computational code is an extension of an early version of the “**Gerris**" code of Popinet (gfs.sf.net). The in-house code implements the following features:

- **Variable-density incompressible Navier-Stokes solver with surface tension**
- **Volume-of-fluid (VOF) interface tracking method with the adaptive mesh refinement**
- **Multi-fluid viscosity model**
- **Balanced-force Continuum Surface Force (CSF) algorithm (extended also to include contact lines)**
- **Height-functions (HF) for accurate computation of normals and curvatures at contact line**

Calculated curvatures at the contact line converge with mesh refinements:

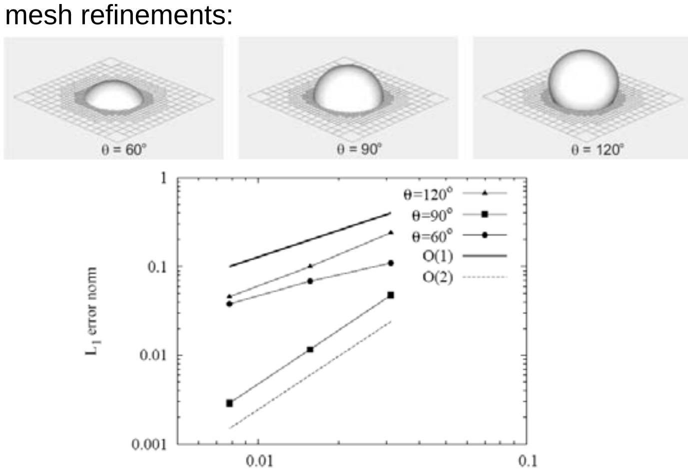

Figure 2: L_1 norm of errors in contact line curvature for drops at equilibrium; $\theta = 60^0, 90^0, 120^0$.

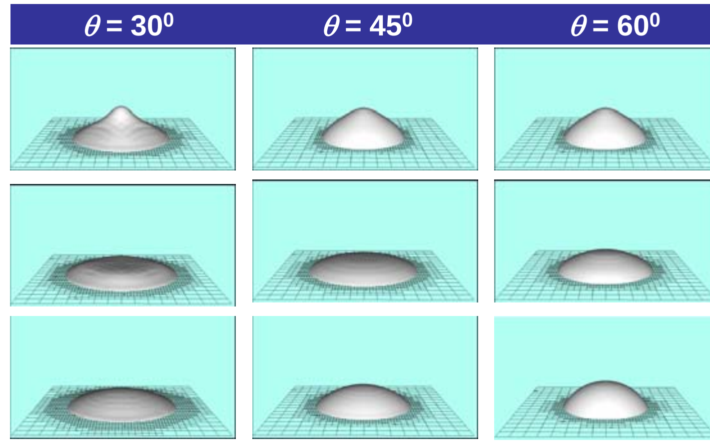

Figure 3: Sequences of droplet shapes. Bottom figures are equilibrium configurations.

An example of a contact line-driven flow is an out-of-equilibrium sessile droplet on a solid surface. An initially hemispherical drop ($\theta = 90^0$) of radius $R = 0.2$ is drawn to a new equilibrium configuration by a sudden change in θ. Imposing a different contact angle will accelerate the drop toward a steady state configuration defined by the new value of θ. **A difficult test of a 3D code for contact line phenomena is its ability to maintain symmetry during an axisymmetric calculation**.

“Electrowetting”

Results in which the contact line drives asymmetric motion are presented. Simulations are presented that illustrate the behavior of a droplet on a surface with a varying contact angle (as in “**electrowetting**”). A hemispherical droplet of radius $R = 200\mu m$ is initially placed at the bottom of a 1*mm* x 1*mm* x 1*mm* domain; the properties are those of water and air. The droplet is at rest ($\theta = 90^0$) when $\theta = 60^0$ (wetting) and $\theta = 120^0$ (non-wetting) are suddenly imposed beneath the two halves of the droplet.

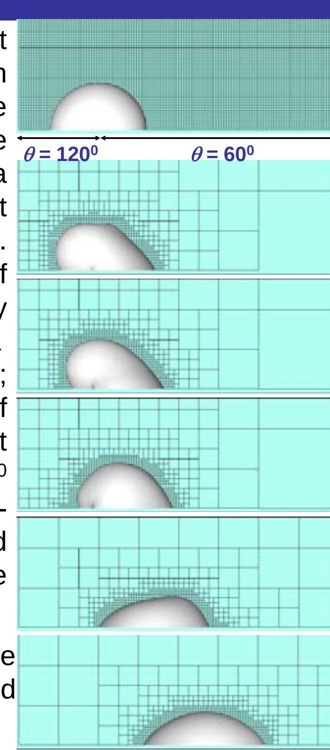

Figure 4: Side views of the droplet, at t = 0, 2, 5, 7, 12, and 30 *ms* (from top to bottom).

Conclusion

We have developed a robust and accurate approach for applying a specified contact angle to VOF simulation, one that leads to accurate predictions of equilibrium configurations.

References:
1- S. Afkhami and M. Bussmann, IJNMF, 57, 453-472, 2008.
2- S. Afkhami and M. Bussmann, IJNMF, 61, 827-847, 2009.
3- S. Afkhami, S. Zaleski, M. Bussmann, JCP, 228, 5370-5389, 2009.

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