A Contact Angle Boundary Condition Derived from Fundamental Hydrodynamics, for the Simulation of Interfacial Flows

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Introduction

The dependence of numerical solutions of moving contact line phenomena on grid-spacing has recently been brought to attention [5, 6, 3, 2]. Here we use a numerical model to demonstrate the scaling of contact line numerical solutions. We show that our model introduces an effective slip through the grid-spacing in the numerical algorithm [3]. We then implement a dynamic contact angle model that is developed based on a hydrodynamic description of the dynamic contact line [1] and that serves as the boundary condition at the moving contact line. This appears to eliminate the contact line singularity and represents a well-posed problem, and results in converged solutions.

Our numerical model is an extension of the "Gerris" code of Popinet [4]. The model employs a volume-of-fluid (VOF) method to track the interface, and a height-function methodology within the "Continuum Surface Force" (CSF) framework for the implementation of the surface tension force. A contact angle is prescribed at the contact line as a boundary condition.

Numerical Results

Consider a liquid pool of dimension L, consisting of two fluids of equal viscosity μ and density ρ, with surface tension σ between them. A solid plate is withdrawn at a constant velocity U_w, in the direction opposite the gravitational acceleration g. The initial Reynolds number $Re = \frac{\rho U_w L}{\mu} = 4$ and capillary number $Ca\frac{\mu U_w}{\sigma} = 0.03$. Simulations are run in a non-dimensional 1x1 domain, with the lower fluid initially at a height of 0.4, at a time step of 1×10^{-5}, to steady state.

A no-slip boundary condition is imposed along the entire solid boundary; our numerical model introduces an effective slip on the scale of the grid size, as per the Navier-slip law. We first show that the numerical solutions depend on grid-spacing, by applying a constant contact angle $\theta = 90$. The results are shown in Fig. 1; Fig. 2 shows interface profiles at different grid resolutions. These results show that the solutions do not converge with grid refinement. In order to evidence the stress singularity, the shear rate along the solid boundary is plotted in Fig. 3. As predicted, shear stress diverges with grid refinement confirming the stress singularity at the contact line.

We now consider a contact angle boundary condition model based on the theoretical analysis of Cox [1]. In Cox's analysis, for a viscous flow ($Re \leq 1$), the macroscopic dynamic contact angle θ_{macro} is related to the molecular contact angle θ_{micro}

$$G(\theta_{macro}) = G(\theta_{micro}) + Ca\ln(\varepsilon^{-1}) + o(Ca) \qquad (1)$$

where ε is the phenomenological slip length and the function G is defined in [1]. Sheng and Zhou [5] showed that Eq. 1 is well approximated by

$$\cos(\theta_{micro}) - \cos(\theta_{macro}) \simeq 5.63Ca\ln(K\varepsilon^{-1}) \qquad (2)$$

where K is a constant depending on the slip model. In our numerical model, θ_{micro} together with θ_{dyn} contribute to the geometric boundary condition for the solution of the macroscopic hydrodynamic equations, where $\theta_{dyn} = F(Ca, \theta_{eq}, ...)$ is the velocity dependent dynamic contact angle and θ_{eq} is the equilibrium contact angle. We first show that the scaling of θ presented by Eq. 2 is demonstrated in our simulations. We vary the contact angle boundary condition θ_{num} so that all the solutions yield the same macroscopic contact angle θ_{macro} at different mesh resolutions. The macroscopic contact angle θ_{macro} is predicted from the interface shape in the numerical simulations. We chose two sets of θ_{num}. In each set, θ_{num} is varied in a manner which yields the same interface deformation at different grid-spacing resulting a similar macroscopic contact angle for all the cases. In Fig. 4, we plot $\cos(\theta_{num}) - \cos(\theta_{macro})$ as a function of the $5.63Ca\ln(K\varepsilon^{-1})$ for $\theta_{num} = 90°$, $84°$, $78°$, $72°$, $63°$ and $\theta_{num} = 114°$, $108°$, $102°$, $97°$, $90°$ corresponding to grid sizes $\Delta = 1/512$, $1/256$, $1/128$, $1/64$, $1/32$. Here, Δ plays the role of the slip length. An excellent fitting curve is obtained by allowing K=0.2 [5]. Our numerical results, therefore, support the validity of our contact angle boundary condition model. As expected, the contact angle increases as the grid-spacing decreases, thereby allowing the surface tension force to balance the stress singularity. Our results also suggest that the contact angle boundary condition θ_{num} scales with the numerical slip length logarithmically.

Closure

We have presented further evidence of the mesh dependence of interfacial flow solutions that involve moving contact lines, and demonstrated a logarithmic dependence of

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the micro-scale contact angle on the slip length that arises from our numerical discretization. On the basis of simulations, we have shown that $\cos(\theta_{num})-\cos(\theta_{macro})$ depends
124 linearly on $Ca \ln(\varepsilon^{-1})$. This scaling relationship can serve as a means to evaluate θ_{num} as a function of grid spacing Δ that yields mesh independent solutions of moving contact line phenomena.

References

[1] R.G. Cox, Inertial and viscous effects on dynamic contact angles, J. Fluid Mech. 357 (1998), 249-278.

[2] M. Latva-Kokko and D.H. Rothman, Scaling of dynamic contact angles in a lattice-Boltzmann model, Phys. Rev. Lett., to be published.

[3] L. Pismen and O. Weinstein, Scale dependence of contact line computations, in 59th Annual Meeting of the APS Division of Fluid Dynamics (2006).

[4] S. Popinet, The Gerris Flow Solver, *http://gfs.sourceforge.net.*

[5] P. Sheng and M. Zhou, Immiscible-fluid displacement: Contact-line dynamics and the velocity-dependent capillary pressure, Phys. Rev. A 45 (1992), 5694-5708.

[6] Y.D. Shikhmurzaev, Singularities at the moving contact line. Mathematical, physical and computational aspects, Physica D: Nonlinear Phenomena 217 (2006), 121-133.

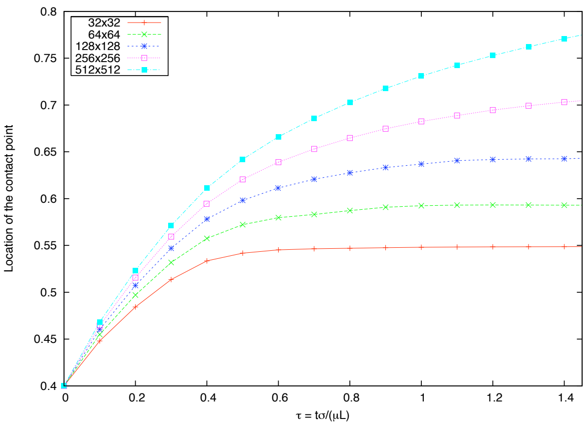

Figure 1: Dependence of the contact line location on grid-spacing, at non-dimensional time τ.

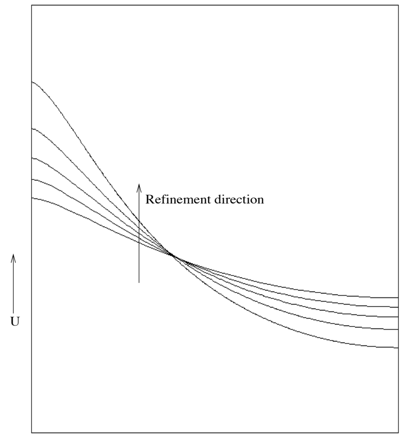

Figure 2: Steady state interfaces at different grid resolutions.

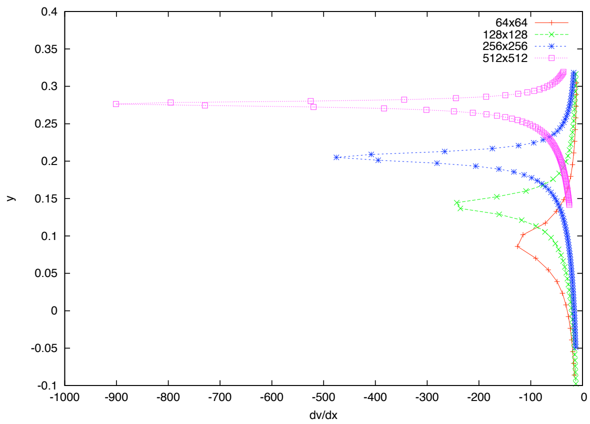

Figure 3: Steady state shear rates at different grid resolutions.

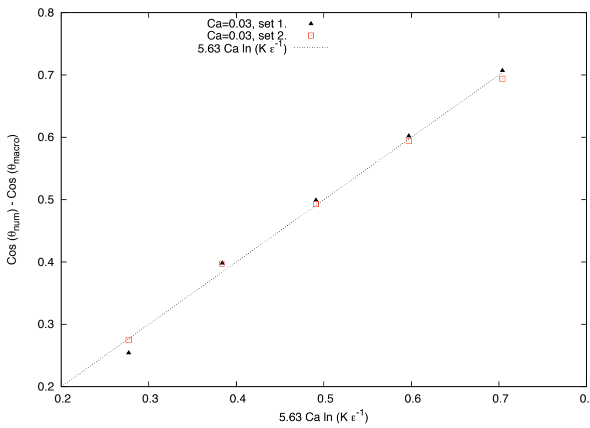

Figure 4: The contact angle boundary condition θ_{num} as a function of the $Ca \ln(K\varepsilon^{-1})$. The dashed line shows the plotted fit using Eq. 2 and $K = 0.2$