Modeling Interfacial Surface Tension in Fluid Flow

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Interfacial flows with surface tension are frequently encountered in nature and in industrial applications, an example being in material processing. Accurately modeling such flows is challenging because of the discontinuity in material properties (such as density) and because of the interfacial boundary condition (surface tension).

As part of the Telluride project, we have developed a balanced-force fluid flow algorithm to accurately model interfacial surface tension effects. The Telluride project is developing the Truchas code, a 3-D finite-volume multi-physics package that models material processes such as gravity casting. Fluid flow is modeled by solving the Navier-Stokes equations on a fixed mesh. The locations of different materials are tracked using the volume tracking method (also know as the volume-of-fluid method), which assumes a single fluid formulation with averaged material properties in a multi-material cell.

Our surface tension model is based on the continuum surface force (CSF) approach of Brackbill et al. [1] in which the interfacial surface force is transformed to a volume force in the region near the interface via a delta function:

$$\vec{F} = (\sigma\kappa\hat{n} + \nabla_s\sigma)\delta$$

where σ is the surface tension coefficient, κ is the mean interfacial curvature, ∇_s is the surface gradient and δ is the delta function. The first term of the equation is acting in the normal direction and the second term in the tangential direction. If the surface tension coefficient is a constant, the tangential component is zero.

The CSF method has the propensity to generate unphysical flow (“spurious currents”) near the interface when surface tension forces are dominant. These spurious currents are best illustrated in the limiting case of an inviscid static drop in equilibrium where Laplace’s formula applies. The causes of these spurious currents are an imbalance of the surface tension and pressure gradient forces and errors in curvature estimations. Therefore, we have devised a balanced-force algorithm [2] such that the normal component of the surface tension force is able to exactly balance the pressure gradient. Because curvatures are proportional to second derivatives of the volume fraction function, it is necessary to smooth the volume fraction to obtain accurate curvatures using a convolution technique or use a more geometrical approach by estimating a height function and discretizing it [2]. Our balanced-force algorithm combined with the convolution curvature method nearly eliminates the spurious currents for the case of the static drop as illustrated in Fig. 1.

We have extended our balanced-force algorithm to model thermocapillary forces that are due to the variation of surface tension coefficient arising from temperature gradients along the interface [3]. Thermocapillary forces are transmitted from the interface to the bulk of the fluid by viscous forces, inducing Marangoni convection in the flow that causes the interface to deform. In our algorithm, the tangential component of the surface tension forces representing the thermocapillary effect is precisely balanced by the viscous stress.

Finally, at rigid boundaries (or wall) we have modified the evaluation of the interfacial normal to represent the contact angle boundary condition as in [1]. Verification of the implementation in Truchas has been achieved by comparison with the analytical results of Sen and Davis [4] for thermocapillary flows in cavities. The steady state results of the simulations are shown in Fig. 2 for a variety of wall adhesion properties (contact angles).

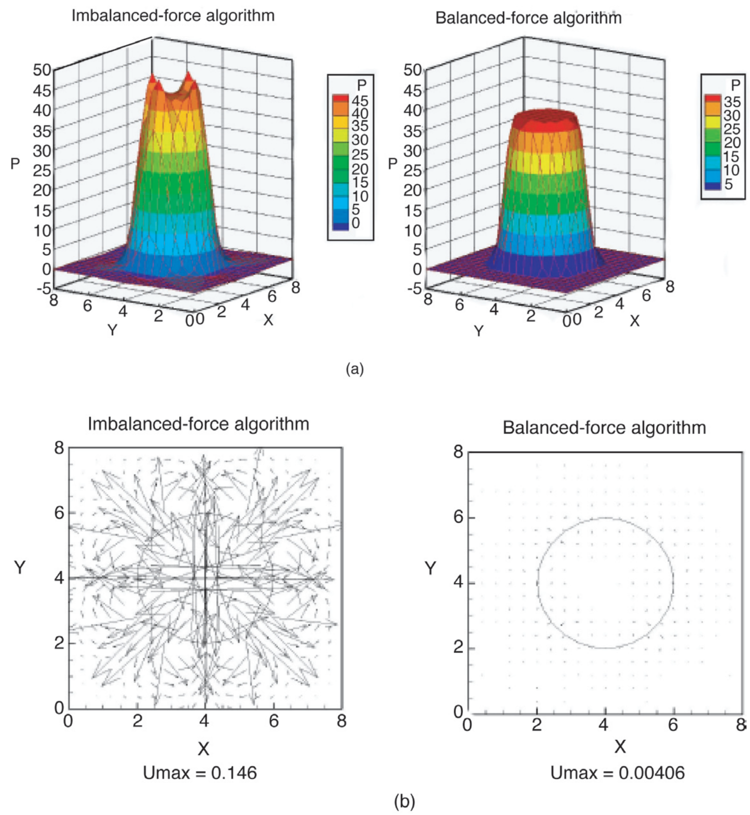

Fig. 1. *Imbalanced vs balanced-force algorithm for the case of an inviscid static drop of radius R = 2 in an 8 x 8 domain with mesh size 20 x 20; (a) pressure distribution and (b) velocity field.*

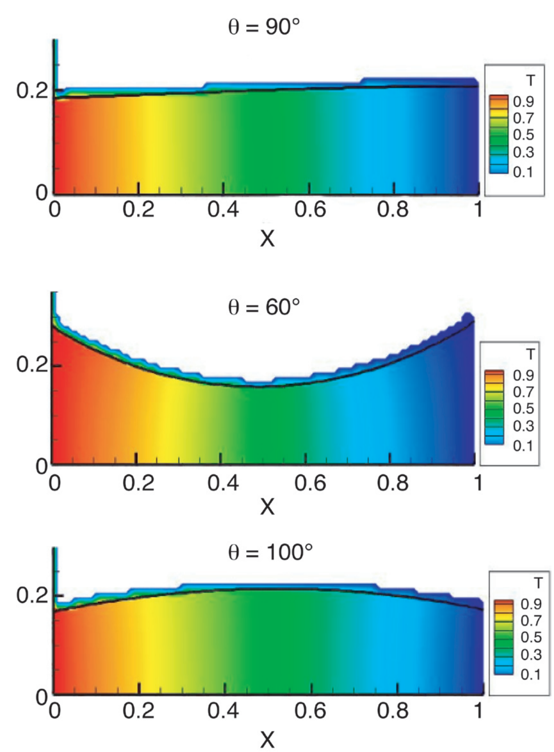

Fig. 2. *Temperature contours and interface shape at steady state for thermocapillary flows in cavities for different contact angle θ. Initially the interface is flat and the cavity aspect ratio is 0.2. The mesh spacing is uniform of 0.02.*

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[2] M.M. Francois, et al., *J. Comp. Phys.* **213**, 141–73 (2006).
[3] M.M. Francois, "Modeling of Thermocapillary Forces Within a Volume Tracking Algorithm," in *Modeling of Casting, Welding and Advanced Solidification Processes—XI,* C.A. Gandin, M. Bellet, Ed. (The Minerals, Metals & Materials Society, 2006) pp. 935–942.
[4] A.K. Sen and S.H. Davis, *J. Fluid Mech.* **121**, 163–186 (1982).

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