Modeling and Simulation of Moving Contact Lines in Multi-phase Flows

(Talk #26)

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I will first discuss a continuum model for moving contact lines derived from principles of non-equilibrium thermodynamics and molecular dynamics simulations. Macroscopic thermodynamic principles are used to place constraints on the form of the boundary conditions, and the detailed constitutive relations are computed from molecular dynamics. This meso-scale contact line model consists of the Navier-Stokes equation, a boundary condition for the slip velocity, and a relation between the dynamic contact angle and the contact line velocity. In the second part of my talk, I will discuss numerical methods for the contact line model, its extension to fluids with surfactants, and contact line motion on patterned surfaces.