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Multiscale modeling of singular cavity flow and moving contact lines[1] XIAOBO NIE, MARK O. ROBBINS, Dept. of Physics and Astronomy, The Johns Hopkins Univ., SHIYI CHEN, Dept. of Mechanical Engineering, The Johns Hopkins Univ. — We have extended our previous continuum-atomistic hybrid method [1] to simulate macro-scale (millimeter and larger) quasistatic flows while retaining atomistic structure in key spatial regions. The method uses local refinement to handle the wide range of spatial scales. The separation in time scales is addressed by iterating the solution at each spatial scale to steady state using smaller time steps at smaller length scales. Speedups of more than 10 orders of magnitude have been obtained compared to pure atomistic simulations. The method has been applied to study wall driven cavity flows with different Reynolds numbers (up to ∼7000) and driving velocities. Singular stresses at the corner lead to an infinite total force on the moving wall in continuum theory. Our hybrid approach allows this force to be investigated for the first time. The method has also has been used to examine similar singularities in motion of the contact line between a fluid interface and a solid wall. The dependence of the dynamic contact angle is evaluated as a function of surface tension, viscosity, system size, and molecular scale slip length and compared to analytic models [2]. 1. X. B. Nie et al, J. Fluid Mech. **500**, 55 (2004); Phys. Fluids **16**, 3579 (2004). 2. R. G. Cox, J. Fluid Mech. **168**, 169 (1886).

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