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Atomistic-continuum hybrid simulations for nano-scale flows PANDURANG KULKARNI, Department of Chemical Engineering, University of California at Santa Barbara, GAURAV TOMAR, Department of Mechanical Engineering, Indian Institute of Science, CHIA-CHUN FU, M. SCOTT SHELL, L. GARY LEAL, Department of Chemical Engineering, University of California at Santa Barbara — It is known that the continuum assumption breaks down when the length scale of a flow approaches few nanometers. Examples include dynamics of thin films and interfaces, slippage in nanochannels and complex biological flows. In this work we develop a hybrid multiscale model, which combines atomistic description in a spatially localized region with continuum description in larger part of the flow domain. The atomistic region is simulated using standard molecular dynamics (MD) with particles interacting via Lennard-Jones pair potential. The continuum part of the problem is solved using the boundary-integral method. The spatio-temporal coupling between the two descriptions is achieved through constrained dynamics in the overlap region. The proposed model is validated by simulating shear flows in channels. A quantitative agreement is found between the computed flow fields and the analytical solutions. The boundary-integral based continuum solver offers improved efficiency and stability over conventional CFD methods. The potential applications of the method in emerging nano-fluidics are discussed.

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