Hybrid simulation of continuum and molecular dynamics for flows over super-hydrophobic surfaces

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Abstract: Micro- and nano-fluidics involve a broad range of scales from the atomic scales to the continuum ones. A full molecular dynamics simulation is able to simulate the fluid flows at the micro- and nano-scales. However, it is computationally prohibitive due to the limitation of computer memory and computation time. On the other hand, a full continuum description, such as the Navier-Stokes equation, is computationally available but unable to describe the fluid flows in the region where the continuum assumption breaks down. A kind of those problems is the superhydrophobics: the patterned roughness on a hydrophobic solid surface enhances its hydrophobics and yields a large slip velocity at the solid surfaces. The superhydrophobics property is particularly attractive, since it may provide an efficient method for mass transport and drag reduction in micro- and nao-fluidics. An appropriate approach to simulate the superhydrophobics is to use the molecular dynamics in one region where the continuum assumption breaks down and use the Navier-Stokes equations in another region where the continuum assumption holds true, and those two descriptions are coupled in the overlap region. The computation time in the hybrid method is expected to be much less than that in the full molecular dynamics simulation. The challenge is how to couple the Navier-Stokes equations with the molecular dynamics simulation. In this talk, I will introduce our recent work on the dynamic coupling model for the hybrid computation and use the hybrid simulation to study superhydrophobics. The numerical issue associated with the hybrid method will be discussed.