Coupled Atomistic-Continuum Methods for the study of Complex Fluids and Micro-Fluidics

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ABSTRACT

In many areas of science and engineering, we face the problem that we are interested in analyzing the macroscale behavior of a given system, but we do not have an explicit and accurate macroscopic model for the macroscale quantities that we are interested in. On the other hand, we do have at our disposal a microscopic model (e.g. molecular dynamics) with satisfactory accuracy - the difficulty being that solving the full microscopic model is far too inefficient.

In this talk, I present a seamless multiscale method, which captures the macroscale behavior of a system with the help of a microscale model. In the seamless algorithm, the micro model supplies the data which is needed but missing in the macro model. The two models evolve simultaneously using their intrinsic time steps, and they exchange data at every time step. We illustrate the multiscale method using examples of complex fluids, in which the macroscopic conservation laws are coupled with molecular dynamics. In the second part of the talk, I discuss the moving contact line problem. The moving contact line problem is a classical problem in fluid mechanics. The difficulty stems from the fact that the classical Navier-Stokes equation with no-slip boundary condition predicts a non-physical singularity at the contact line with infinite rate of energy dissipation. In this talk, I show how continuum theory and molecular dynamics can be combined to give us a better understanding of the fundamental physics of the moving contact line and formulate simple and effective models. I also illustrate how this model can be used to analyze hysteresis and other important physical problems for the moving contact line.

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