Constrained variation in multiscale simulations of micro- and nano-fluidics and subgrid-scale stress model of fluid turbulence

Shiyi Chen
College of Engineering, Peking University

Abstract

Finding physically consistent solutions in multiscale methods is crucial for various multiscale modeling and simulations. A framework for continuum and molecular dynamics hybrid multiscale method has been recently developed to simulate micro- and nano-fluid flows. In this approach, the continuum Navier-Stokes equation is used in one flow region and atomistic molecular dynamics in another. The spatial coupling between two methods is achieved through the constrained dynamics in an overlap region. The proposed multiscale method has been validated in simple fluid flows, including sudden-start Couette flow and channel flow with nano-scale wall roughness, showing quantitative agreement with results from analytical solutions and full molecular dynamics simulations. The hybrid method is then used to study the singularity problems in the driven cavity and moving contact lines. Following the stress over more than six decades in length in systems with characteristic scales of millimeters and milliseconds allows us to resolve the singularity and determine the force for the first time. The speedup over pure atomistic calculation is more than fourteen orders of magnitudes.

The similar idea of constrained variation has also been used for developing constrained dynamic subgrid-scale (C-SGS) stress model of fluid turbulence. In the C-SGS, we impose physical constraints in the dynamic procedure of calculating the SGS coefficients. In particular, we study dynamics mixed models with energy flux and helicity flux constraints. The comparison between the large eddy simulation results in steady and decay isotropic turbulence using constrained and non-constrained SGS models and those from direct numerical simulation (DNS) will be presented. It is found that the C-SGS not only predicts the turbulent dissipation more accurately, but also shows a strong correlation between the model stress and the real stress from a priori test, which is a desirable feature combing the advantages of dynamics Smagorinsky and traditional mixed models.