2012 Special Program in Applied Mathematics and Applied Mechanics

Dissipative particle dynamics (DPD) on fluid constitute modeling

2012 - 02 - 29 (Wed.)
10:30 - 12:00
101, Mathematics Research Center Building (ori. New Math. Bldg.)

The dissipative particle dynamics is a mesoscopic particle based simulation method. The basic unit in DPD system is a set of discrete momentum carriers (particle) in continuous space and discrete time steps. Unlike the molecular dynamics simulation (MD), the particles in DPD are supposed to represent the fluid on a mesoscopic level rather than at a molecular level. The motion of DPD particles is governed by Newton's equations of motion and the interaction between particles are assumed to be pairwise. In our studies, the pairwise force applied on the DPD particles can be divided into three parts, the conservative force, the dissipative force and the random force. In order to increase the Schmidt number (the ratio of the dynamics viscosity to diffusion constant), the weight function of the forces were modified. The simple shear flow was simulated to verify the DPD methods, the velocity profile, shear stress and the differences of normal stress were investigated. Concerning the non-Newtonian fluid, certain numbers of dumbbells with linear spring force were allocated in the DPD particles to simulate the Oldroyd-B fluid. The relationships between the difference of normal stress and viscosity versus shear rate and relaxation time versus concentration and stiff constant were studied. The fluid within single or multi droplets were also simulated with current DPD methods. Some results on the fluid stress as well as the motions of droplets will be shown.