CENTER FOR FLUID MECHANICS AND THE FLUIDS, THERMAL AND CHEMICAL PROCESSES GROUP OF THE DIVISION OF ENGINEERING SEMINAR SERIES

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Fluctuating Immersed Material (FIMAT) Dynamics for the Direct Numerical Simulation of the Brownian Motion of Particles

A Direct Numerical Simulation (DNS) scheme, named Fluctuating Immersed MATerial (FIMAT) dynamics, for the Brownian motion of rigid particles will be presented. In this approach the thermal fluctuations are included in the fluid equations via random stress terms. Solving the fluctuating hydrodynamic equations coupled with the particle equations of motion result in the Brownian motion of the particles. There is no need to add a random force term in the particle equations. The particles acquire random motion through the hydrodynamic force acting on its surface from the surrounding fluctuating fluid. The random stress in the fluid equations is easy to compute unlike the random terms in the conventional Brownian/Stokesian Dynamics type approaches. The approach is tested for a variety of cases including single spheres, single ellipsoids and many spheres by considering quasi-steady simulations in the long time limit. Translational and rotational diffusion of the particles are considered. Unsteady simulations are also performed to test the short time behavior of the velocity autocorrelations. The method correctly reproduces the algebraic tail of the velocity autocorrelation.

TUESDAY – March 14, 2006 Barus & Holley, Room 190 3:00pm