CFD BASED ON FLUCTUATING FLUID DYNAMICS FOR SUB-MICRON/NANOSCALE APPLICATIONS

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The interaction of sub-micron/nanoscale objects (such as macromolecules or small particles or small devices) with fluids is one of the key problems encountered in miniaturized systems. Various physical phenomena should be modeled simultaneously for a fundamental investigation of small scale devices. We are working on a novel and fundamental methodology to simulate the Brownian motion of objects in sub-micron/nanoscale devices.

A particle suspended in a fluid experiences a hydrodynamic force due to the average motion of the fluid around it. The average motion of the fluid is represented by the usual continuum equations such as the Navier-Stokes equations. Small particles in fluids, in addition to the average force, experience a random force due to the thermal fluctuations in the fluid. In conventional Brownian Dynamic simulations the principle is to model this thermal force from the fluid in terms of a random term in the particle equation. We adopt a different approach where the thermal fluctuations are modeled in the fluid itself via random stress and heat flux terms in its governing equations. The properties of these random stresses are determined by the fluctuation-dissipaton theorem. The coupled fluid-particle equations are then solved to obtain the Brownian motion of the particles. The coupled fluid-particle problem can be solved by a Distributed Lagrange Multiplier (DLM)/fictitious domain method.

We will discuss the formulation and the numerical implementation of this problem. Advantages of this approach over the conventional approach will be addressed.