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A Lattice Boltzmann-Direct Forcing/Fictitious Domain Model for Brownian Particles in Fluctuating Fluids

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Abstract. The previously developed LB-DF/FD method derived from the lattice Boltzmann method and Direct Forcing/Fictitious Domain method is extended to deal with 3D particle's Brownian motion. In the model the thermal fluctuations are introduced as random forces and torques acting on the Brownian particle. The hydrodynamic interaction is introduced by directly resolving the fluid motions. A sphere fluctuating in a cubic box with the periodic boundary is considered to validate the present model. By examining the velocity autocorrelation function (VCF) and rotational velocity autocorrelation function (RVCF), it has been found that in addition to the two relaxation times, the mass density ratio should be taken into consideration to check the accuracy and effectiveness of the present model. Furthermore, the fluctuation-dissipation theorem and equipartition theorem have been investigated for a single spherical particle. Finally, a Brownian particle trapped in a harmonic potential has been simulated to further demonstrate the ability of the LB-DF/FD model.

AMS subject classifications: 68U20, 76T20, 76M28, 82B80

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1 Introduction

Particles suspended in fluids experience a random force due to the thermal fluctuations in the fluid around them in addition to the average hydrodynamic force. Brownian motion

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may take place for those sub-micron/nanoscale particles. For many applications in microsystems for chemical and biological analysis, the ability to control and measure temperature inside microfluidic devices is critical since temperature often affects biological or chemical processes. Recent developments [1,2] demonstrate that the well-defined temperature dependence of the Brownian motion of nanoparticles could be used to present a temperature measurement technique which offers several benefits over existing methodologies. Brownian particle can be adopted to measure the local viscoelastic response of soft materials [3] or the topography of a surrounding polymer network [4]. The motion of a Brownian probe can also be used to characterize mechanical properties of molecular motors by analyzing the particle's trajectory [5]. Moreover, the biased Brownian motions or rectified Brownian motions, induced by an energy source [6] or by broken spatial reflection symmetry [7], provide a very effective technique for particle separation. Furthermore, it has been demonstrated [8,9] that nano-particles in a conventional base fluid, known as nanofluids, tremendously enhance the heat transfer characteristics of the original fluid. At the same time, many groups [10–12] have declared that Brownian motion is a key mechanism governing the thermal behavior of nanofluids. Besides, the theory of stochastic processes originated from Brownian motion have found wide applications in climate dynamics [13], stock market [14], traffic flow [15] and so on, which should go beyond Einstein's first consideration. Due to its importance in engineering applications, there has always been a great deal of interest in developing algorithms that can provide a better understanding of particle's Brownian motion. Especially in some cases [3–5], high resolution of Brownian motion is needed, which requires the numerical algorithms have the ability to observe the motion on short time scales ($t \ll \tau_D$, $\tau_D = a^2/D_0$, a is the spherical particle radius, D_0 is the particle diffusion coefficient).

Roughly speaking, the existing numerical methods for modeling particle's Brownian motion can be categorized by the treatment of particle's motion equations into three groups. (1) Langevin-type equation based method. Brownian dynamics (BD) [16] and Stokes dynamics (SD) [17,18] are the most important methods in this group. These methods treat the particle's motion by the Langevin equations without treatment of the fluid flow which indicates that random fluctuations are applied directly into the particles. For BD approximate expressions are used to model the hydrodynamic interactions and for SD the Rotne-Prager-Yamakawa tensors are used to express the hydrodynamic interactions. BD and SD are widely used numerical methods and achieved great success in the simulations of particles' Brownian motion. One of limitations of these methods may be that they cannot account for the short-time motion [19]. (2) DNS (Direct Numerical Simulation) method. In this group, the thermal fluctuations in the fluid, which result in the Brownian motion of particles, are modeled by adding a random stress tensor to Navier-Stokes equations. This method was called fluctuating hydrodynamics [20]. Solving the fluctuating hydrodynamic equations coupled with the particle equations of motion result in the Brownian motion of particles. In this method, the particles acquire random motion through the hydrodynamic force acting on its surface from the surrounding fluctuating fluid. Therefore, there is no need to add a random force term in the particles'