Thermal equilibrium of a Brownian particle in a fluctuating fluid: a numerical study

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Abstract. In this work the fluctuating lattice Boltzmann method was adopted to simulate the motion of a Brownian particle in a fluid in two dimensions. The temperatures characterizing the translation motion and rotational motion of the particle were calculated to evaluate the thermal equilibrium between the particle and the fluid. Furthermore, the effects of the fluid temperature and viscosity on the fluid pressure fluctuation were investigated. The linear relationships were observed in a log-log coordinate. Besides, the slopes of the linear relation were obtained, which keeps constant for all cases studied.

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 may take place for those sub-micron/nanoscale particles. For many applications in microsystems, 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, study [10] has declared that Brownian motion is a key mechanism governing the thermal behavior of nanofluids. 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.

The most important and accurate approach to simulate particle Brownian motion may be the fluctuating hydrodynamics, which was proposed by Landau and Lifshitz [11]. In this approach, 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. Solving the fluctuating hydrodynamic equations coupled with the particle equations of motion result in the Brownian motion of particles. As a direct numerical simulation scheme, there is no need to add a random force term in the particles’ equations since random fluctuations are applied directly to the particles.
The thermal equilibrium between the Brownian particles and the fluids is quite fundamental to the modelling particle Brownian motion, which has been paid little attention in the past. Therefore, in this work the fluctuating dynamics was used to simulate the motion of a Brownian particle in two dimensions. The present work aims to study the thermal equilibrium between the particle and the fluid, as well as the pressure fluctuation.

2. Numerical Model

The fluid flow is solved by the LB method. The discrete LB equations of a single-relaxation-time model are described as [12],

\[ f_i(x, c_i, \Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau} [f_i(x, t) - f_i^{(0)}(x, t)] + f_i'(x, t) \]  

(1)

where \( f_i(x, t) \) is the distribution function on the i-direction microscopic velocity \( e_i \), \( f_i(0)(x, t) \) is the equilibrium distribution function, \( \Delta t \) is the time step of the simulation, \( f_i'(x, t) \) is a stochastic term representing the thermal fluctuations, which is related to the fluctuating stress in the Navier-Stokes equation [12]. The fluid density \( \rho \) and velocity \( \mathbf{u} \) are determined by the distribution function,

\[ \rho = \sum_i f_i, \quad \rho \mathbf{u} = \sum_i f_i \mathbf{e}_i \]  

(2)

For the two-dimensional D2Q9 lattice model used here, the discrete velocity vectors are,

\[ e_i = \{(\pm 1, 0)c, (0, \pm 1)c, \quad \text{for } i = 1 \text{ to } 4, \]  
\[ (\pm 1, \pm 1)c, \quad \text{for } i = 5 \text{ to } 8, \]

where \( c = \Delta x / \Delta t, \Delta x \) is the lattice spacing. The equilibrium distribution function is chosen as,

\[ f_i^{(0)}(x, t) = \omega_i \rho \left[ 1 + \frac{3e_i \cdot u}{c^2} + \frac{9(e_i \cdot u)^2}{2c^4} - \frac{3u^2}{2c^2} \right] \]  

(3)

As shown by Nie and Lin [12], the stochastic term is related to the fluctuating stress,

\[ \sigma_{i\beta}' = -\tau \sum_j f_i' e_{i\beta} \]  

(4)

According to the fluctuation-dissipation theorem, has the following property [11],

\[ \langle \sigma_{i\beta}' \rangle = 0 \]  

(5)

\[ \langle \sigma_{i\beta}'(x, t) \sigma_{i\beta}'(x, t') \rangle = 2k_B T \mu \left( \delta_{i\beta} \delta_{ij} + \delta_{ij} \delta_{i\beta} \right) \delta(\mathbf{x} - \mathbf{x}_j) \delta(t - t_j) \]

where <> denotes averaging over an ensemble, \( k_B \) is the Boltzmann constant, \( T \) is temperature of the fluid, \( \mu \) is the dynamic viscosity of the fluid. The fluctuating stress is sampled from a Gaussian distribution with zero mean and a given variance of \( 2k_B T \mu \).

In this work we assume the stochastic term \( f_i'(x, t) \) to be the following form to make sure of the conservation of mass and momentum [12],

\[ f_i' = 0 \]

\[ f_i' = f_i' = \frac{1}{2\tau} \sigma_{i\beta}' \]

\[ f_i' = f_i' = \frac{1}{\tau^2} \sigma_{i\beta}' \]

\[ f_i' = f_i' = \frac{1}{4\tau} \left( \sigma_{i\beta}' + \sigma_{i\beta}' + \sigma_{i\beta}' \right) \]

\[ f_i' = f_i' = \frac{1}{4\tau} \left( \sigma_{i\beta}' + \sigma_{i\beta}' - \sigma_{i\beta}' \right) \]  

(6)

3. Results and Discussion

In this work, the Brownian motion of a single particle in a periodic domain was numerically investigated. Only the hydrodynamic force was considered. The periodic domain is 256×256 in the simulations, which is large enough to eliminate the effect of boundary. The density of the fluid is \( \rho = 1 \) and the non-dimensional relaxation time \( \tau = 0.8 \), which leads to the fact that the viscosity of the fluid is \( \nu = 0.1 \). The radius of particle is \( a = 3.5 \). The solid/fluid density ratio is \( \rho_s / \rho = 11 \). In order to
determine the magnitude of the fluid fluctuation, the variance of fluctuating stress is chosen as $2k_B T \mu = 10^{-4}$. It should be stated that all the above-mentioned parameters are in lattice unit.

In Fig. 1, the instantaneous velocity field of fluid is shown at different times, along with the Brownian particle. As shown in the figure, the velocity vectors are disorderly and disorganized, which represents the random molecular motion of the fluid. This is the origin of the Brownian motion of particle in a fluid, which is resulted from the essence of the present fluctuating lattice Boltzmann method. As one can see in Fig. 1, the particle moves randomly due to the fluid molecular collision. This suggests that it is impossible to predict the motion of particle, such as the velocity or the trajectory of particle. In addition, the rotation of particle is also attained in the simulation, which is different from the Langevin dynamics.

![Figure 1](image1.png)

Figure 1. Instantaneous flow for a Brownian particle suspended in a fluctuating fluid: (a) $t = 10000$, (b) $t = 50000$, (c) $t = 100000$, (d) $t = 200000$

Fig. 2 shows the pressure fluctuation of fluid at different times, which also presents the disorderly and disorganized results. As shown in the figure, the pressure fluctuation is randomly but homogeneously distributed in the whole domain. Undoubtedly, the results shown in Fig. 1 and Fig. 2 reveal the microstructure of fluid in a very simple way.

![Figure 2](image2.png)

Figure 2. Instantaneous pressure for a Brownian particle suspended in a fluctuating fluid: (a) $t = 10000$, (b) $t = 50000$, (c) $t = 100000$, (d) $t = 200000$

It has been shown that thermal equilibrium between the Brownian particle and the surrounding fluid molecular will reach and that an equipartition of energy for each degree of freedom will be observed, which can be described as

$$
\langle U^2 \rangle = \langle V^2 \rangle = k_B T / M, \langle \Omega^2 \rangle = k_B T / J
$$

(7)

where $U$ and $V$ refer to the translational velocity of $x$ and $y$ coordinate, respectively, and $\Omega$ refers to the rotational velocity of particle. $M$ and $J$ are the mass and inertial of the particle, respectively. An equipartition of energy for $x$ and $y$ translational motion can be observed, as well as the rotational motion, as displayed in Fig. 3, which shows the thermal equilibrium of $Re = 0.035$ and $Re = 0.15$, respectively.

The temperatures characterizing translational motion of $x$ and $y$ coordinate, and the rotational motion agree with each other after a certain time, but all about 5% less than or more than the effective temperature of the fluid, as on can see in Fig. 3. The similar results were also obtained by Ladd [13], which are however 15% less than the effective temperature of the fluid.
Fig. 3. Time history of normalized mean square of translational/rotational velocity: (a) $Re=0.035$, (b) $Re=0.15$

Fig. 4 summarizes the temperatures representing the translational and rotational velocity of a Brownian particle for different Reynolds number. All the results shown in the figure are normalized, which demonstrates that the difference between the particle temperature and the fluid temperature is within 5%. As a result, the thermal equilibrium between the Brownian particle and the fluctuating fluid is almost achieved irrespective of the Reynolds number.

Fig. 5. The pressure fluctuation as a function of: (a) the fluid temperature and (b) viscosity
Fig. 6 shows the normalized translational and rotational velocity correlation functions, which are the fundamental results of a Brownian particle. As shown in the figure, all the results are decaying to zero, indicating that the velocity of Brownian particle become more unrelated for larger time interval. In addition, the similar rate of decay is observed for both horizontal and vertical components. The rotational velocity correlation function is decaying faster than that of translational velocity.

![Figure 6. The translational and rotational velocity correlation functions](image)

4. Conclusion
In this work a fluctuating lattice Boltzmann model was adopted to simulate the Brownian motion of a particle in two dimensions. Results show that the difference between the particle temperature and the fluid temperature is within 5% irrespective of the Reynolds number, indicating the thermal equilibrium is almost achieved. Moreover, it has been shown that the pressure fluctuation has a linear relationship with the fluid temperature in a log-log coordinate. The slope is shown to be about 0.5 for all cases. Similar feature is observed for the relationship between the pressure fluctuation and the fluid viscosity.

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