Direct coupling between molecular dynamics and lattice Boltzmann method based on velocity distribution functions for steady-state isothermal flow

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ABSTRACT

The direct coupling scheme between the molecular dynamics (MD) and lattice Boltzmann method (LBM) is established in this paper. Different from the existing coupling schemes which are based on the exchange of the density and velocities, the proposed coupling scheme is based on the velocity distribution functions. Firstly, the relations between the discrete velocity distribution functions of LBM and the continuous velocity distribution functions of MD are derived based on the Hermite expansions. Then, the coupling schemes between MD and LBM are proposed. The inconsistency between the equation of states of MD and LBM is specially treated and the deviatoric stresses are exchanged. The coupling simulations of the Poiseuille flow and Couette flow demonstrate that both the velocity and stress can be well exchanged by the coupling scheme. The coupling simulation of the flow past a nanotube shows that the proposed method can be further used in the study of microscopic fluid flow problems.

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1. Introduction

Due to the development of the micro-electro-mechanical systems (MEMS), the fluid flow and heat transfer in micro-/nano-scale have drawn a lot of attentions. When the characteristic lengths of the fluid flow and heat transfer problems are comparable to the mean free path of the molecules, new phenomena such as the velocity slip and temperature jump occur [1]. These phenomena are different from the assumptions and descriptions of the continuum models. In order to simulate and predict these phenomena, the molecular dynamic (MD) simulation is widely employed. Since the MD simulation has to deal with the motion of each molecules, it consumes much more computational resources than the continuum approaches. Therefore, the hybrid or coupling models are proposed to couple the MD with the traditional numerical methods to increase its efficiency [2,3]. In the hybrid methods, the computational domain is decomposed. The MD is only applied in the area where it is necessary and in the rest of the domain the continuum method is used to save the computational time. The information of the MD and continuum methods are exchanged at the interfaces [4].

In the recent years, the lattice Boltzmann method (LBM) has been rapidly developed. The LBM is based on the kinetic theory, which is between the macroscopic continuum models and the microscopic molecule motions. Therefore, it is a mesoscopic method and it can be a bridge between the macroscopic method and the molecular methods [5]. Consequently, many works has been done to couple the LBM with the macroscopic and microscopic methods to establish the multiscale numerical methods [6–16]. Although the coupling between LBM and macroscopic/mesoscopic methods has been widely studied [7–12], the coupling between LBM and the microscopic MD method still needs further studies. Therefore, in this work we focus on the coupling between MD and LBM.

It should be mentioned that there are other kinds of hybrid numerical methods. For example, the MD can be applied separately to get the interfacial tension, wettability and other properties of the fluid systems, and then the properties are adopted in the multiphase LBM models [17]. In the other field-wise coupling schemes, the continuum methods are applied in the whole computational region and the MD is used as the correction and refinement for the constitutive laws and boundary conditions of the continuum methods [18,19]. These coupling methods are difference from the coupling method in this paper. Here the coupling method is based on the domain decomposition. The LBM and MD are applied

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simultaneously in different regions, and the information exchange between them is the key problem of the method.

In the existing researches about the coupling between LBM and MD, Dupuis et al. [13,14] proposed a hybrid LBM-MD model for the simulation of dense fluids. The Schwarz alternating method is used to decouple the time scales of the MD and LBM. At the LBM boundary, a forcing term is added to the governing equation to impose the velocity boundary condition from MD to LBM. This approach is either adopted in a one-cell-wide strip (velocity-coupling) or all the common area (velocity-gradient-coupling). At the MD boundary, the molecular velocities relax to the desired velocities given by the LBM with a small relaxation parameter. The flow past a carbon nanotube (CNT) is simulated and the results of the coupling method agree well with the reference MD solutions. Neumann et al. [15] developed the parallel MD-LBM software based on the similar method. Zhou et al. [16] also coupled LBM with MD. In their simulation, the reconstruction operator, which is proposed for the coupling between LBM and macroscopic methods, is used at the LBM boundary to convert the velocity and density into the distribution functions of LBM. For the inverse information transfer, the velocities of the molecules in the boundary areas are reset according to a Maxwell distribution which is obtained from the velocities and temperatures of the LBM simulation.

In the above coupling strategies, the variables transferred between MD and LBM are only density and velocities. However, both the MD and LBM contain more information than these variables. For example, the velocities of each molecule and the interaction between each pair of molecules are known in MD. In the LBM, the density distribution functions of each discrete velocity are known, which can give not only the local density and velocities, but also the local stress tensor. Therefore, if only the density and velocities are transferred, the information is lost and not sufficiently used. There should be a coupling strategy which directly links the micro-/meso-scale and transfers information more sufficiently. This kind of coupling method can also give more insights between the LBM and MD.

There are some existing coupling schemes that also take into consideration of the stress tensor. For example, Delgado-Buscalioni and De Fabritiis coupled MD with fluctuating hydrodynamics, in which the stress calculated in the MD is transferred to the continuum method by a flux coupling [20]. Di Staso et al. coupled LBM with Direct Simulation Monte Carlo (DSMC) [11,12]. The Hermite expansions are used for the transformation between continuous and discrete velocity distribution functions. Due to the similarity between DSMC and MD, this coupling scheme has the potential to be further extended to the coupling between LBM and MD.

Therefore, in the present work, we try to extend the direct coupling method via the velocity distribution functions proposed by Di Staso et al. [11,12] to the case of coupling between MD and LBM. In the rest of the paper, the MD and LBM are briefly reviewed in Sections 2 and 3. In Section 4, based on the velocity distribution functions, the coupling scheme between LBM and MD is established. Then, the numerical tests of the coupling scheme are conducted in Section 5. Finally, some conclusions are given in Section 6.

2. Molecular dynamics simulation

In the molecular dynamic, the motion of every molecule is calculated. For the classical molecular dynamics, the motion of the molecule is described by Newton's second law as

$$m_0 \ddot{\mathbf{r}}_i = \mathbf{f}_i \tag{1}$$

in which m_0 is the mass of a molecule, $\mathbf{r}_i$ is the location of the ith molecule and $\mathbf{f}_i$ is the force acting on that molecule, which contains the interaction between molecules and the external forces. The Lennard-Jones (L-J) potential is used in this work to describe the interactions. The potential φ is a function of the distance, $r = |\mathbf{r}_i - \mathbf{r}_j|$, between two molecules as [21]

$$\varphi(r) = 4\varepsilon \left\{ \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] + \left[6 \left(\frac{\sigma}{r_c} \right)^{12} - 3 \left(\frac{\sigma}{r_c} \right)^{6} \right] \left(\frac{r}{r_c} \right)^{2} \right.$$
$$\left. - \left[7 \left(\frac{\sigma}{r_c} \right)^{12} - 4 \left(\frac{\sigma}{r_c} \right)^{6} \right] \right\} \tag{2}$$

Here σ and ε govern the interaction length and strength of the potential. r_c is the cutoff distance for the potential and we chose $r_c = 2.5\sigma$. In the computation, it is assumed that there is no interaction between a pair of molecules when the distance between them is larger than r_c. The second and third term in the brace can guarantee the continuous of the potential and force at $r = r_c$. The interaction force that molecule j exerts on i is

$$\mathbf{f}_{ij} = -\frac{\partial \varphi(r)}{\partial \mathbf{r}_i} = -\frac{\partial \varphi(r)}{\partial r} \frac{(\mathbf{r}_i - \mathbf{r}_j)}{r} \tag{3}$$

Therefore, the force acting on a molecule is the summation of all the interaction force on it and the external force $\mathbf{f}_i^e$ as

$$\mathbf{f}_i = \sum_j \mathbf{f}_{ij} + \mathbf{f}_i^e \tag{4}$$

In the present work, for convenience, the following dimensionless variables are used in the MD simulations:

$$r = r_{MD}\sigma, \tag{5}$$

$$t = t_{MD}\sqrt{m_0 \sigma^2 / \varepsilon} \tag{6}$$

$$v = v_{MD}\sqrt{\varepsilon/m_0} = v_{MD}\sqrt{k_0 T_0 / m_0} = v_{MD} v_0 \tag{7}$$

$$m = m_{MD} m_0 \tag{8}$$

$$T = T_{MD}\varepsilon/k_0 = T_{MD} T_0 \tag{9}$$

$$E = E_{MD}\varepsilon \tag{10}$$

In the above equations, r, t, v, m, T and E denote the length, time, velocity, mass, temperature and energy. k_0 is the Boltzmann constant. The variables with the subscript MD are dimensionless variables, and the variables with subscript 0 denote scales. We will ignore the subscript MD in the rest of the paper and the dimensionless values of MD are used in all the following problems.

In order to obtain the macroscopic values, the computational region in MD are divided into several cells. Then, the macroscopic values of each cell are calculated by the ensemble average of the molecules inside the cell. However, the system size for LBM simulations can be pushed down to one molecule per cell [22]. Therefore, instead of just using a spatial average, a temporal average over an interval δt^M should be also applied in each cell. For the non-steady-state simulations, the δt^M should be much smaller than the characteristic time scale of the problem. For the steady-state problems considered in this work, a sufficiently long δt^M is chosen to control the statistical errors in each cell. For example, the macroscopic density ρ, velocity $\mathbf{u}$, stress tensor $\mathbf{P}$ and temperature T are calculate by

$$\rho_{MD} = \left\langle \frac{N}{V} \right\rangle_{\delta t^M} \tag{11}$$

$$\mathbf{u}_{MD} = \left\langle \frac{1}{N} \sum_{i=1}^{N} \dot{\mathbf{r}}_i \right\rangle_{\delta t^M} \tag{12}$$