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Coupling MD particles to a lattice-Boltzmann fluid through the use of conservative forces

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ABSTRACT

We propose a new method for coupling both point and composite MD particles to a lattice-Boltzmann fluid. This coupling is implemented through the use of conservative forces, calculated by assuming elastic collisions between the particles and the fluid, thereby eliminating the need for any adjustable coupling constants. With the implementation of a mass and momentum conserving thermal lattice-Boltzmann method, the fluid acts as a heat bath for the MD particles without the need for external Langevin noise. We demonstrate the effectiveness of this method using a variety of simple, well known flow problems. In addition, by studying the velocity autocorrelation function, we are able to validate the fluctuation–dissipation theorem for the algorithm.

1. Introduction

The lattice-Boltzmann algorithm [1,2] is a popular method used to simulate the hydrodynamics of complex fluids on a grid. As this method requires only nearest neighbour grid point information, it is very straightforward to implement, and is ideally suited for large-scale parallel applications. Recently, it has become increasingly popular to use this method in conjunction with molecular dynamics simulations, to model situations where the dynamics of the MD particles depend on the hydrodynamic interactions between them. The resulting coupled lattice-Boltzmann, MD algorithms have been applied to a range of situations, including colloidal suspensions [3], blood flow [4,5], polymers in solution [6–8], DNA translocation [9], and flow through disordered media [10,11], and colloidal particles in a liquid crystal [12].

Several different methods have been introduced to treat the coupling between the lattice-Boltzmann fluid, and the MD particles. The original approach of Ladd [12,13] treated the interaction via a set of bounce-back rules at boundary nodes placed halfway along the links between fluid nodes cut by the particle surface. This has proven an effective method for large particles, however discrepancies in the hydrodynamic behavior, dependent on the relaxation time of the LB fluid, occur for radii smaller than $\sim 2.4\Delta x$ [3].

As an alternative, Alrichs and Dünweg [14] used a frictional force proportional to the local velocity difference between the particle and the fluid, to couple point particles to the lattice-Boltzmann fluid. In order to use this type of method for a larger particle, a representation of that particle in terms of point particles is required. Peskin et al. [15–17] have worked extensively on the treatment of such representations, creating the immersed boundary method to incorporate moving boundaries into a fluid; however, for a somewhat different application than discussed here. Composite particles were first modeled in the lattice-Boltzmann framework using the force-coupling method by Lobaskin and Dünweg [18].

In order to model a particle in a fluctuating lattice-Boltzmann fluid using the frictional force-coupling method, Alrichs and Dünweg [14] found they required the addition of external Langevin noise to the forces in order for the particle motion to

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obey the fluctuation dissipation theorem consistent with the temperature of their fluid. This was justified by the dissipative nature of the coupling force. Here, we remove the question of the need for external Langevin noise, by introducing a new force coupling method which uses conservative forces. With this coupling method, the fluid alone acts as a heat bath for the particles. The theoretical details of our method are described in Section 2, while Section 3 provides various tests of the method.

2. Theoretical background

2.1. The lattice-Boltzmann algorithm

The fluid motion in our system is governed by the continuity and Navier–Stokes equations,

$$\partial_t \rho + \partial_\beta(\rho u_\beta) = 0,$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = \partial_\beta \sigma_{\alpha\beta} + F_\alpha + \partial_\beta\left(\eta_{\alpha\beta\gamma\nu}\partial_\gamma u_\nu\right), \tag{1}$$

where ρ is the fluid density, u_α is the velocity, $\sigma_{\alpha\beta}$ is the stress tensor, F_α is a local external force, and $\eta_{\alpha\beta\gamma\nu}$ is the viscosity tensor,

$$\eta_{\alpha\beta\gamma\nu} = \eta\left[\delta_{\alpha\gamma}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\gamma} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\gamma\nu}\right] + \Lambda\delta_{\alpha\beta}\delta_{\gamma\nu}. \tag{2}$$

Here, η represents the shear viscosity, and Λ, the bulk. For the work presented here, we set $\sigma_{\alpha\beta} = -\rho a_0 \delta_{\alpha\beta}$, where a_0 represents the square of the speed of sound in the fluid.

To solve these equations on a discrete grid of points we use a lattice-Boltzmann algorithm. This algorithm utilizes a velocity discretized version of the linearized Boltzmann equation, implemented here as a finite difference scheme,

$$f_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{\Delta t}{\tau}\left[f_i(\mathbf{x}, t) - \left[f_i^{eq}(\mathbf{x}, t) + \tau W_i(\mathbf{x}, t)\right]\right] \tag{3}$$

in order to solve for the motion of a set of partial distribution functions, $[f_{i=1,\ldots,N}]$, with each f_i corresponding to a discrete velocity direction, $\mathbf{e}_i$. These partial distribution functions can be thought of as direction specific fluid densities, with moments given by:

$$\begin{aligned}\rho &= \Sigma_i f_i,\\ \rho u_\alpha &= \Sigma_i f_i e_{i\alpha}.\end{aligned} \tag{4}$$

We use an implementation of the algorithm in which each grid point is connected to its neighbouring points by a set of $N = 15$ velocity directions (D3Q15), with velocity vectors given by

$$\mathbf{e}_i = (0,0,0),\ (\pm v_c, 0, 0),\ (0, \pm v_c, 0),\ (0, 0, \pm v_c),\ (\pm v_c, \pm v_c, \pm v_c). \tag{5}$$

Here $v_c = \Delta x/\Delta t$, and Δx, and Δt are the lattice spacing, and the timestep respectively.

Eq. (3) uses the BGK [19] model for the Boltzmann collision term, with τ, which is physically related to the viscosity in the fluid, representing the single time relaxation parameter, and f_i^{eq} corresponding to the local equilibrium distribution functions. External forcing terms are introduced through the functions, W_i.

In order to enforce conservation of mass, momentum, and to control the stress tensor in the system, the equilibrium distributions are chosen according to

$$\begin{aligned}\Sigma_i f_i^{eq} &= \rho,\\ \Sigma_i f_i^{eq} e_{i\alpha} &= \rho u_\alpha,\\ \Sigma_i f_i^{eq} e_{i\alpha} e_{i\beta} &= \sigma_{\alpha\beta} + \rho u_\alpha u_\beta,\end{aligned} \tag{6}$$

while the forcing terms, W_i, which control the external force F_α are chosen to satisfy

$$\begin{aligned}\Sigma_i W_i &= 0,\\ \Sigma_i W_i e_{i\alpha} &= F_\alpha,\\ \Sigma_i W_i e_{i\alpha} e_{i\beta} &= u_\alpha F_\beta + F_\alpha u_\beta.\end{aligned} \tag{7}$$

With these constraints, a Chapman–Enskog expansion performed on Eq. (3) can be shown to reproduce Eq. (1), with viscosities given by

$$\begin{aligned}\eta &= \rho\left(\tau - \frac{\Delta t}{2}\right)v_c^2/3,\\ \Lambda &= \eta(5/3 - 3a_0/v_c^2).\end{aligned} \tag{8}$$