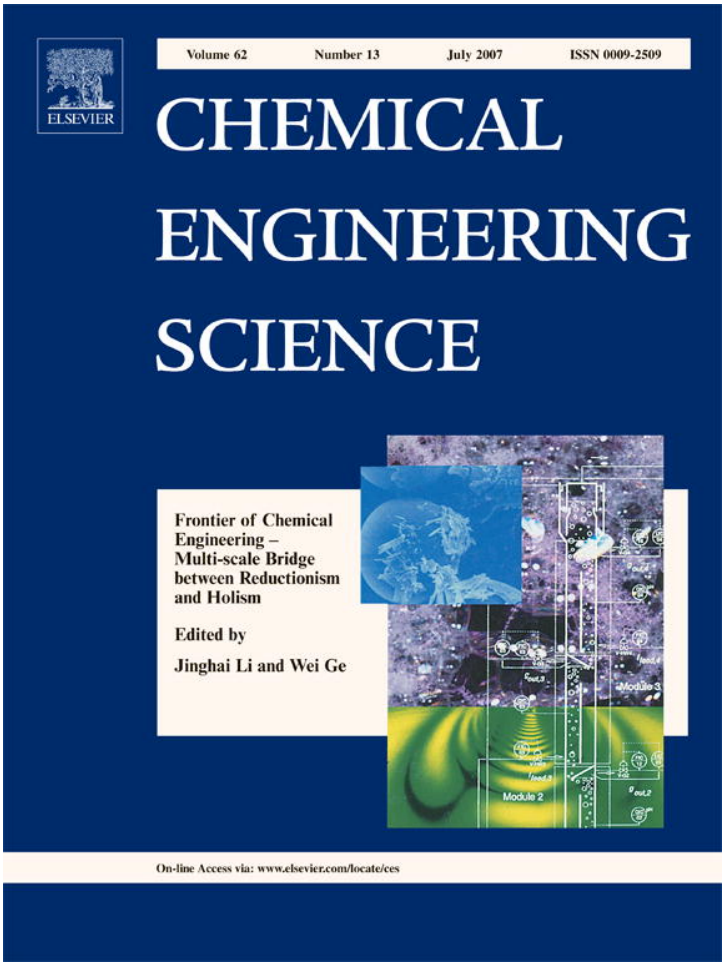

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A dynamic coupling model for hybrid atomistic–continuum computations

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Abstract

A dynamic coupling model is developed for a hybrid atomistic–continuum computation in micro- and nano-fluidics. In the hybrid atomistic–continuum computation, a molecular dynamics (MD) simulation is utilized in one region where the continuum assumption breaks down and the Navier–Stokes (NS) equations are used in another region where the continuum assumption holds. In the overlapping part of these two regions, a constrained particle dynamics is needed to couple the MD simulation and the NS equations. The currently existing coupling models for the constrained particle dynamics have a coupling parameter, which has to be empirically determined. In the present work, a novel dynamic coupling model is introduced where the coupling parameter can be calculated as the computation progresses rather than inputing *a priori*. The dynamic coupling model is based on the momentum constraint and exhibits a correct relaxation rate. The results from the hybrid simulation on the Couette flow and the Stokes flow are in good agreement with the data from the full MD simulation and the solutions of the NS equations, respectively.

PACS: 47.85.Np; 47.11.−j; 02.70.−c; 68.08.−p

Keywords: Dynamic coupling; Hybrid method; Microfluidics; Molecular dynamics

1. Introduction

The problems in microfluidics involve a broad range of scales from the atomistic scale to the continuum one (e.g. see Squires and Quake, 2005; Gad-el-Hak, 2004). A full atomistic description, such as molecular dynamics simulation, is capable of describing the fluid flows at the micro- and nano-scales. However, it is computationally prohibitive due to the limitations of computer memory and computational time. On the other hand, A full continuum description, such as the Navier–Stokes (NS) equations, is computationally available but unable to describe the fluid flows in the regions where the continuum assumption breaks down. One of those examples is the slip boundary condition on fluid–solid interfaces (see Thompson and Troian, 1997; Pit et al., 2000). In order to take the advantages of both the atomistic and continuum descriptions, a hybrid atomistic–continuum method (e.g. see O'Connell and Thompson, 1995; Li et al., 1998; Nie et al., 2004; Koumoutsakos, 2005; Cui et al., 2006) has been recently developed. In the hybrid method, an atomistic description is combined with a continuum one, see Fig. 1. It describes the fluid as an amount of particles in one region where the MD is used, and as a continuum hydrodynamics in another region where the NS equations are used. These two descriptions are coupled in the overlap region. Thus, the boundary conditions for the NS equations, which are not explicitly available at micro- and nano-scales, can be obtained from the MD simulations. Meanwhile, the macroscopic information on the NS equations is given to the molecules via the interactions of the particles with the molecules. The computation time in the hybrid method is expected to be much shorter than the full MD computation in the entire domain, since most of the computation region is solved by the NS equations. The challenge is how to couple the continuum dynamics with the MD to ensure the continuity of the physical quantities, such as mass, momentum, energy and their fluxes, in the overlap region. Unlike the previous hybrid method in turbulent reacting flows (see Muradoglu et al., 2001), which is a particle-then-continuum approach, the present one is a particle-and-continuum approach.

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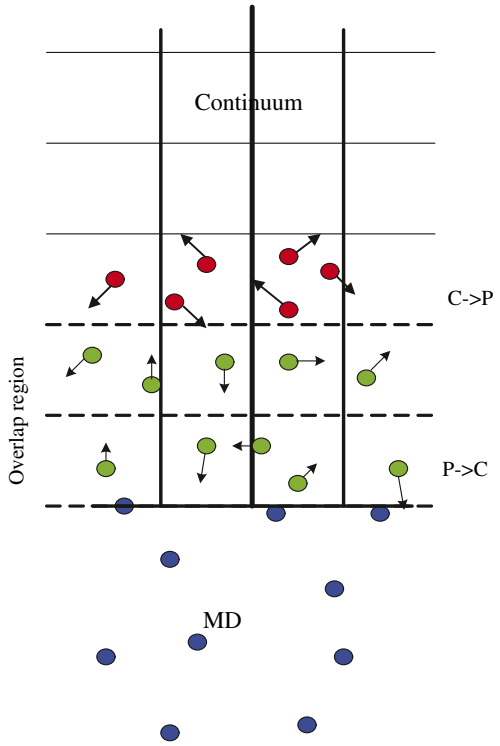

Fig. 1. A schematic diagram for the hybrid method. Circles indicate the particle region; Straight lines indicate the continuum region. $C \rightarrow P$ is the upper surface of the particle region and $P \rightarrow C$ is the lower surface of the continuum region. The overlap region is in between the two surfaces.

There are two coupling approaches available: the flux-based method (e.g. see Delgado-Buscalioni and Coveney, 2003) or the state-based method (e.g. see Hadjiconstaniou and Patera, 1997). The flux-based coupling makes the fluxes of mass, momentum and energy calculated from the MD and the NS *equations*, respectively, consistent. In the overlap *region*, the fluxes calculated from the MD simulation are exchanged with the ones calculated from the NS equations. Therefore, the coupling model can naturally satisfy the conservation laws. Unfortunately, the coupling may induce some numerical instability due to the Dirichilet problem. Flekkoy et al. (2000) developed a robust flux-based coupling model. Their results demonstrate some advantages over the state-based method; The state-based coupling is to transfer the state information between the MD simulation and NS equations. In the overlap region, a constrained particle dynamics is constructed and serves as a bridge to transfer the information so that the averaging of particle information gives a macroscopic state to the NS equations and the macroscopic information from the NS equations iss given to the particles. The particles interact with molecules in the atomistic region and thus transfer the information into the molecules.

O'Connell and Thompson (1995) developed a constrained particle dynamics with an empirical coupling parameter. In their computations, the coupling parameter is taken as 0.01 *a priori*. Recently, Nie et al. (2004) proposed a modification of *O'Connell and Thompson's* model using an external force. It implies that the coupling parameter is equal to unity. These coupling models have been used to successfully simulate the sudden-started Couette flows. However, in the simulation, the coupling parameter has to be given a priori. There is no any general approach to determine the coupling parameter to date. In the present work, a dynamic coupling model is proposed to locally calculate the coupling parameter for describing the state of flow in the overlap region. This will be achieved by invoking the momentum consistence constraint.

The paper is organized as follows: in Section 2, the dynamic coupling model for the coupling parameter will be presented and its properties discussed. The dynamic coupling model is tested against the sudden-started Couette flows and the Stokes flow (oscillatory shear flows). The results of these tests will be presented in Section 3. The concluding remark will be made in Section 4.

2. A dynamic coupling model in the hybrid method

We consider a hybrid atomistic–continuum method for micro- and nano-fluidics. In the hybrid method, a computation domain is decomposed into three regions: an atomistic region where a MD is used, a continuum region where the NS equations are used and an atomistic–continuum overlap region to which a constrained particle dynamics is applied. The constrained particle dynamics has to be constructed so that the particle description is consistent with both atomistic and continuum descriptions.

We start with the continuum region. In the region, the NS equations for incompressible flows are used

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u}. \tag{2}$$

Here, $\mathbf{u}$ is the velocity of fluid, ρ the density, $\mathbf{p}$ the pressure and ν the kinematic viscosity. A two-dimensional flow in the x–z plane is considered and the NS equations are numerically solved using the projection method on the stagger grids (e.g. Tannehill et al., 1997), see Fig. 2.

In the atomistic region, the MD simulation is implemented (e.g. see Frenkel and Smit, 1996). The molecular interaction

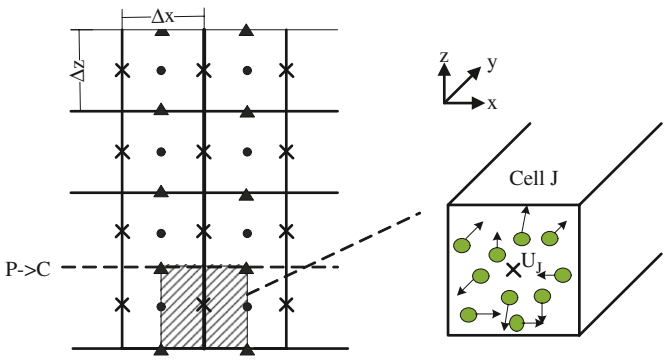

Fig. 2. A schematic diagram for the staggered grids in the continuum region. Crosses and triangles indicate the x and z components of the velocities, respectively. Δx and Δz are the length of the grid in x and z directions. Dashed lines denote the cells where the boundary conditions for the NS equations aree needed.

potential is given by a shifted Lennard–Jones (LJ) potential truncated at $r = r_c$

$$V^{LJ} = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6 - (\sigma/r_c)^{12} + (\sigma/r_c)^6], \tag{3}$$

where ε and σ are the characteristic energy and length scale separately. r_c is a cutoff length, which implies that the interactions vanish when the particle separations are larger than r_c. Then, the equation of motion for each molecule is

$$m_i \frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = -\sum_{j\neq i} \frac{\partial V_{ji}}{\partial \mathbf{r}_i}. \tag{4}$$

The equations of motion are integrated using the Verlet scheme. The temperature of the fluid is maintained to be constant, which is achieved by a Langevin thermostat.

In the overlap region, a constrained particle dynamics is constructed in order to achieve the mass and momentum consistencies between the atomistic and continuum descriptions. The momentum consistence implies that the local mean of the particle momentum is equal to the instantaneous macroscopic momentum

$$\langle m_i v_i \rangle = M_J u_J, \tag{5}$$

where m_i is the mass of the ith particle in the Jth cell, v_i the ith particle velocity, M_J the total mass of the fluid in the Jth cell and u_J the fluid velocity in the Jth cell. The symbol "$\langle\ \rangle$" denotes an ensemble average. In order to achieve the momentum consistence, we start the constrained particle dynamics with the conventional Newton equation for particles

$$\frac{\mathrm{d}^2\mathbf{x}_i}{\mathrm{d}t^2} = \frac{\mathbf{F}_i}{m_i}, \tag{6}$$

where $\mathbf{x}_i$ is the displacement of the particle i. The force, $\mathbf{F}_i$, is determined by the LJ potential

$$\mathbf{F}_i = -\sum_{j\neq i} \frac{\partial V_{ij}^{LJ}}{\partial \mathbf{r}_i}. \tag{7}$$

According to the Langevin equation, an external force is introduced in Eq. (7) to take into account the velocity difference between the particle velocity and the macroscopic velocity. Thus, Eq. (6) can be written as

$$\frac{\mathrm{d}^2\mathbf{x}_i}{\mathrm{d}t^2} = -\frac{1}{m}\frac{\partial V_{ji}}{\partial \mathbf{x}_i} + \xi\left(u_J - \frac{1}{N_J}\sum_{j=1}^{N_J}\frac{\mathrm{d}\mathbf{x}_j}{\mathrm{d}t}\right). \tag{8}$$

Here, N_J is the total number of particles in the Jth cell. ξ is a parameter for coupling intensity, which controls the relaxation of the particles in the overlap region to the local continuum values. Other Langevin-type models include O'Connell and Thompson's model and Nie et al.'s model. In O'Connell and Thompson's model, the coupling parameter is taken as $\xi = 0.01$ to guarantee the relaxation of the local mean of the particle velocity to the macroscopic velocity over some time scale; Nie et al.'s model implies $\xi = 1.0$, which constrains the local mean of the particle velocity equal to the instantaneous macroscopic velocity. An appropriate value of the coupling parameter is critical to the hybrid method.

In order to determine the coupling coefficient, we sum up Eq. (8) over the Jth cell and then solve it for the parameter ξ:

$$\xi_J(t+\Delta t) = \frac{\frac{1}{N_J}\sum(\mathrm{d}^2 r_i(t)/\mathrm{d}t^2 - F_i(t)/m)}{u_J(t) - (1/N_J)\sum_{J=1}^{N_J} v_i(t)}. \tag{9}$$

The coupling parameter obtained might be different in each cell and at each time step. It is dynamically determined by the current states and does adjust the particle dynamics themselves as the computation progresses. Therefore, the dynamic coupling model satisfies the constraint on momentum consistence, and controls the relaxation rate of the local mean of the particle momentums to the macroscopic momentum.

We argue that the coupling parameter ξ must be positive. If the velocity difference $u_J - (1/N_J)\sum \mathrm{d}\mathbf{x_i}/\mathrm{d}t$ is positive, the coupling parameter has to be positive to accelerate the particles, and on the other hand, if the velocity difference is negative, the coupling parameter has to be positive to decelerate the particles. Therefore, we may take the magnitude of the coupling parameter in practice. This ensures the convergence of the results from the MD portion to the ones from the continuum portion.

Mass continuity can be achieved by moving particles across the boundary of the overlap region. Since mass change only happens in the thin layer near the boundary, we define a constrained layer adjacent to the interface between the continuum region and the particle region. In this layer, a certain number of particles are inserted into or removed from the MD region according to the mass flux evaluated by the NS equations. The number of particles that should be inserted or removed across the boundary is

$$n = -A\rho u_z \Delta t_{FD}/m, \tag{10}$$

where A is the area of the cell boundary that are perpendicular to the interface and $\triangle t_{FD}$ is the time step for integrating the NS equations. If n is positive, n particles are inserted into the regular intervals over the time unit $\triangle t_{FD}$. They are placed near the interface in z direction and randomly in x and y directions. To prevent the distance between the inserted particles and the previous ones from being too small, we will repeat the above process if it happens. The initial velocities of these inserted particles are equal to the continuum velocity at the surface to ensure that the average of particle velocities is consistent with the macroscopic velocity. If n is negative, n particles that are closest to the interface are removed. At each interval $\triangle t_{FD}$, the nearest integer of n is taken.

Furthermore, in order to obtain the continuity of momentum flux near the interface, an external force in z direction should be imposed to the particles in the constrained layer. The sum of those external forces in a cell should be determined by the following equation:

$$\sum_i F_i' = A\left(-P + 2\mu\frac{\partial u_z}{\partial z}\right). \tag{11}$$

Here, F_i' is the external force acting on the ith particle, P the local pressure and u_z the velocity in z direction obtained

by solving the NS equations. Eq. (11) indicates that the forces on the particles in the constrained layer are determined by the continuum dynamics. To prevent the particles from flying away from the MD region, we introduce a force F_i' as follows:

$$F_i' = \frac{g(z^i)}{\Sigma_{j\in V} g(z^j)} F. \tag{12}$$

Here, F denotes the right-hand side of Eq.(11) and $g(z_i)$ is an arbitrary weight function which depends on the particle's position in z direction. The function should guarantee that the external force for each particle at the interface C → P is approaching infinite and the one for each particle on the bottom surface of the constrained layer is equal to zero. Thus, the particles are effectively constrained in the MD region.

3. Numerical results

The hybrid method developed in the last section is first used to simulate a sudden-start Couette flow in order to demonstrate its validity. The Couette flow with non-slip boundary conditions is often served as a benchmark test to validate various hybrid methods. Further, we will consider the Couette flows with slip boundary conditions. Finally, we will apply the hybrid method to an oscillatory shear flow, since the oscillatory induced unsteadiness is a challenge to the hybrid method.

The parameters in our simulation are given as follows: the mass of each fluid atom is m, the density $\rho=0.81m\sigma^{-3}$, the cut-off length $r_c=2.2\sigma$. The characteristic time $\tau=(m\sigma^2/\varepsilon)^{1/2}$, the temperature of the fluid is kept constant at $T=1.1\varepsilon/k_B$, where k_B is Boltzmann's constant, the damping rate of the Langevin thermostat is τ^{-1}, and at these given T and ρ, the fluid is in a well-defined liquid phase with viscosity $\mu=2.14\varepsilon\tau\sigma^{-3}$.

The Couette flow is the viscous fluid confined between two parallel plates, with its initial velocity equal to zero. At $t=0$, the top plate at $z=H=46.9\sigma$ is moving with a velocity $U_w=\sigma/\tau$ in x direction and the bottom one at $z=0$ is fixed, see Fig. 3. The sudden-start Couette flow is simulated in a rectangle domain of $46.9\sigma\times46.9\sigma$ in the x–z plane. A periodic boundary condition is imposed in the streamwise direction. In the hybrid method, the computation domain in $0\leqslant x\leqslant46.9\sigma$ and $0\leqslant z\leqslant H$ is divided into two regions: the upper one at $15.63\sigma\leqslant z\leqslant H$ is the continuum region which is described by the NS equations with 9×6 uniform grids $\Delta x\times\Delta z=5.21\sigma\times5.21\sigma$, and the boundary condition at $z=15.63\sigma$ of the NS equations is taken from the results of MD; the lower one at $0\leqslant z\leqslant31.26\sigma$ is the particle region which is described by MD, with extending one grid to $y=4.81\sigma$ in the spanwise direction; the overlap region at $15.63\sigma\leqslant z\leqslant31.26\sigma$ is solved by the constrained particle dynamics described in the last section.

Standard no-slip conditions are imposed at the top wall, while the bottom wall at $z=0$ is simulated by two (1 1 1) layers of a face-centered cubic (FCC) lattice consisting of solid particles with the same mass and density as the liquid. Those particles are fixed in the MD simulations and interact with fluid particles in terms of a shifted LJ potential. The LJ potential with the characteristic energy $\varepsilon^{wf}=0.6\varepsilon$, length scale $\sigma^{wf}=1.0\sigma$ and characteristic density $\rho^{wf}=1.0\rho$ yields a non-slip boundary condition; the LJ potentials with the parameters $(\varepsilon^{wf},\sigma^{wf},\rho^{wf})=(0.6\varepsilon, 0.75\sigma, 4\rho)$ and $(0.2\varepsilon, 0.75\sigma, 4\rho)$ yield two different slip boundary conditions (Thompson and Troian, 1997).

The time step used in the MD portion is $\Delta t_{MD}=0.005\tau$, while in the NS region we use $\Delta t_{NS}=50\Delta t_{MD}=0.25\tau$. The time coupling scheme in the overlap region is shown in Fig. 4. First, $n_p=50$ time steps in the MD are conducted, then the average is performed over the time interval and the averaged information is transferred to the NS equations at the center point of the interval; then, the NS equations are advanced for one time step and the information is sent to the MD, where the extrapolation of velocity field may be needed.

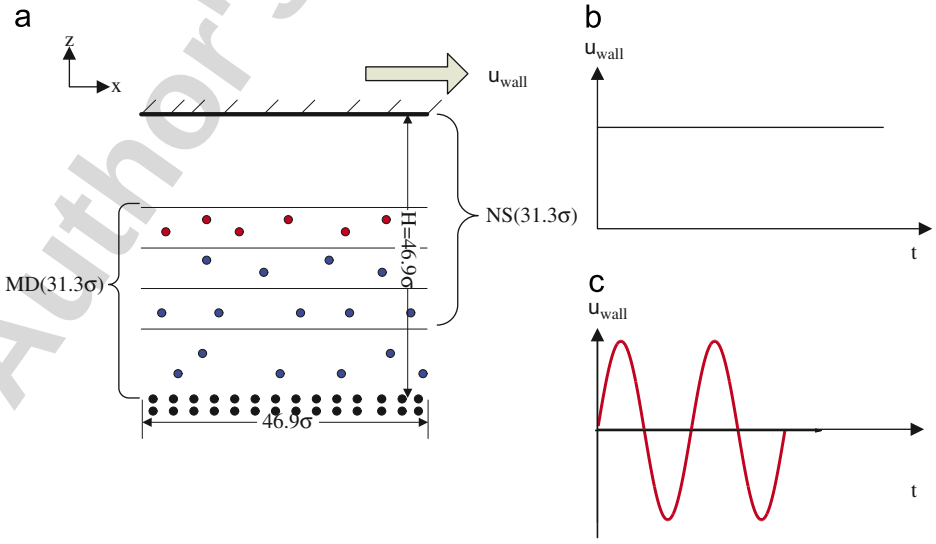

Fig. 3. A schematic diagram of the flows simulated. (a): The geographic configuration, H denotes the distance between the two plates. The two lines of circles in the bottom represent the solid substrate. U_{wall} is the moving velocity of the top plate in the x direction;(b): sudden-start Couette flow where U_{wall} is constant;(c): oscillatory flow where U_{wall} evolves in a sinusoidal way.

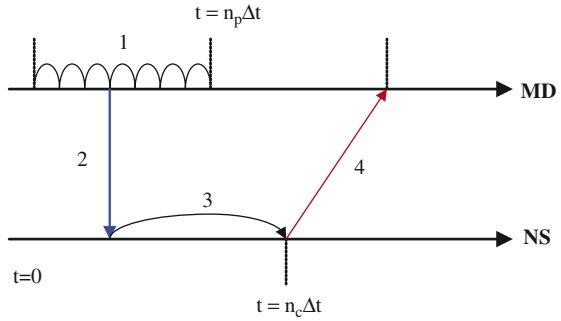

Fig. 4. Time coupling in the hybrid scheme. (1). MD advances n_p time steps; (2) the averaging of n_p steps of MD results gives the information of the center moment to NS; (3) NS advances n_c steps; (4) the NS results give the information to MD, then MD evolves n_p steps again, note that NS can only provide the information up to the middle point of the interval.

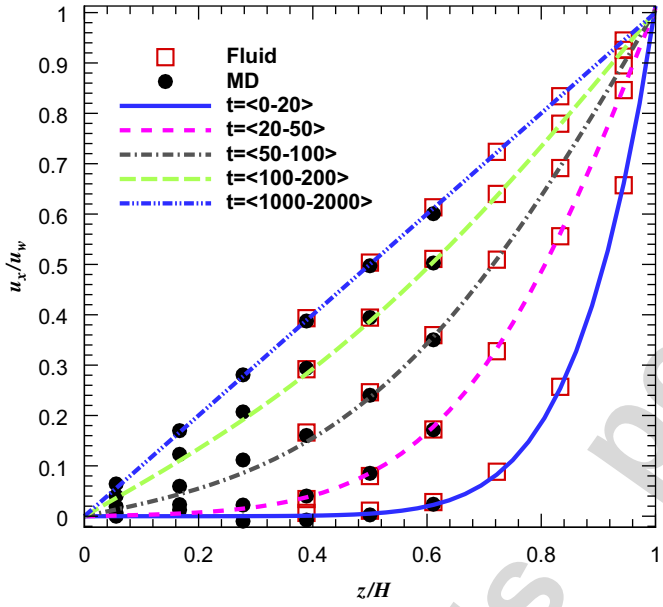

Fig. 5. Velocity profiles at different times from the hybrid method and analytical solutions of the Navier–Stokes equations. Lines denote the analytical solution from the Navier–Stokes equations; empty squares denote the result in the continuum region and solid circles denote the one in the particle region.

The overlap region has three cells in the normal direction and the constrained layer consists of the cells nearest to the interface $C \rightarrow P$. In the continuum region, the projection method is used. We first run the simulation in the MD region for 200τ to a relatively steady state from the initial positions and velocities. The hybrid simulations run for 2000τ to achieve a steady state.

Fig. 5 shows the solutions of the sudden-start Couette flow with the non-slip boundary conditions, using the hybrid method and the analytical solution of the NS equations separately. To reduce the statistical errors in the hybrid method, we average the solutions for 10 independent runs. It can be seen that the results from the hybrid method follow the ones from the analytical solutions. Especially, in the overlap region, the velocities obtained from the NS equations and the MD are smoothly connected. This indicates that the constrained particle dynamics achieves the continuity of the momentum flux. We also implement the hybrid method with constant coupling parameters. The results obtained are dependent on its values. It is not possible to pick up the appropriate coupling parameter a priori.

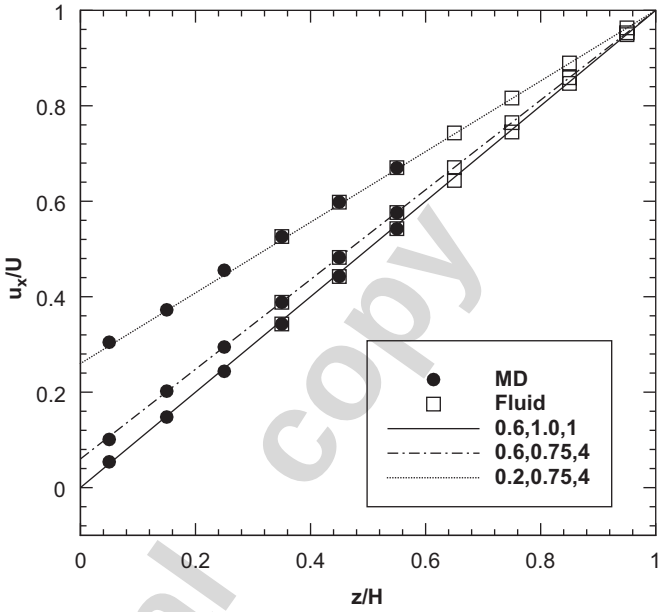

Fig. 6. Steady velocity profiles of the Couette flows under the non-slip and slip boundary conditions. The inlet indicates the symbols of the results obtained from the hybrid method and full MD computation.

Fig. 6 shows the steady solutions of the sudden-start Couette flows with two different slip boundary conditions at the bottom plate. It can be seen that the hybrid scheme reproduced the MD solution very well. The different slip velocities at the bottom plates do induce the velocity profiles of different slopes, which are in good agreement with the previous predictions (Thompson and Troian, 1997). It is verified that the hybrid method developed here is valid for the slip boundary conditions.

To test the dynamic coupling model against unsteady flows, we examine an incompressible and isothermal fluid in an oscillatory shear field between two parallel walls. The lower wall is again kept at zero velocity and the upper wall moves at a sinusoidal speed

$$u(H,t) = u_{\text{wall}}(t) = u_{\max}\sin(2\pi f t). \tag{13}$$

This flow has a analytical solution (Wijmans and Smit, 2002). At large t, the solution can be expressed as

$$u(z,t) = A u_{\max}\sin(2\pi f t + \phi), \tag{14}$$

where

$$A = \left\{\frac{\cosh(2z\sqrt{\pi f/\nu}) - \cos(2z\sqrt{\pi f/\nu})}{\cosh(2H\sqrt{\pi f/\nu}) - \cos(2H\sqrt{\pi f/\nu})}\right\}^{1/2} \tag{15}$$

and

$$\phi = \arg\left\{\frac{\sinh\left(z(1+i)\sqrt{\pi f/\nu}\right)}{\sinh\left(H(1+i)\sqrt{\pi f/\nu}\right)}\right\}. \tag{16}$$

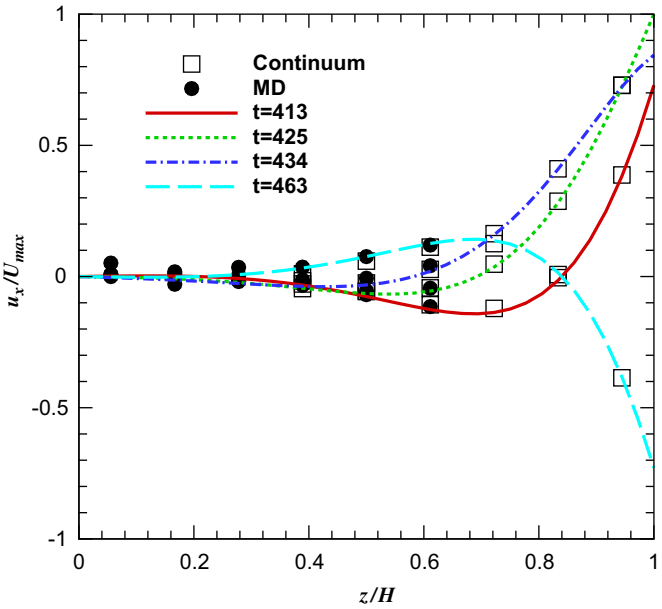

Fig. 7. Velocity profiles for oscillatory flow. Lines denote the analytical solution; symbols denote the hybrid result, empty squares denote the result in the continuum region and solid circles denote the one in the particle region. The unit of time is τ.

Here, $i=\sqrt{-1}$, f is a frequency; arg denotes phase angle complex argument. The set-up here is same as the sudden-Couette flow illustrated above, but the wall moves at the velocity in Eq. (13). An average is performed over a time interval τ that is centered at the specific moment. Besides, we ran 10 realizations of the same system in parallel to reduce the statistical fluctuations. Fig. 7 shows several snapshots of the velocity profiles in the case of $u_{\max}=\sigma/\tau$ and $f=0.01$. Although the velocities slightly fluctuate in the pure MD region, the agreement between the velocity profiles from the hybrid method and the analytical solutions *is* remarkable, which demonstrates the capability of the hybrid method for unsteady flows. Note also that the atomistic and continuum portions of the solution obtained match closely in the overlap region. The hybrid method allows the coupling parameter to evolve with the particle dynamics, which guarantees the relaxation rate.

4. Concluding remarks

A dynamic coupling model has been developed for the hybrid atomistic–continuum computation. The coupling model is based on a Langevin equation. It is "dynamic" in the sense that it is able to calculate the coupling parameter as computation progresses. Therefore, the dynamic coupling model can ensure the continuity of momentum and control the relaxation rates of the systems under investigations.

Two problems are simulated using the dynamic coupling model: the Couette flow and the Stokes flow. The Couette flow tests the dynamic coupling model against its relaxation to the steady states. The Stokes flow tests the dynamic coupling model against the unsteady properties. The results obtained show good agreement with the analytical solutions and the MD simulations. More test cases are needed to investigate the properties of the dynamic coupling model, such as the wall with roughnesses in the Couette flow and Stokes flow with a broad range of frequencies and amplitudes. Other state-based or flux-based constraints can be also utilized to determine the coupling parameter for different purposes.

Acknowledgments

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