RESEARCH PAPER

A constrained particle dynamics for continuum-particle hybrid method in micro- and nano-fluidics

Jia Cui · Guo Wei He · Dewei Qi

Abstract   A hybrid method of continuum and particle dynamics is developed for micro- and nano-fluidics, where fluids are described by a molecular dynamics (MD) in one domain and by the Navier–Stokes (NS) equations in another domain. In order to ensure the continuity of momentum flux, the continuum and molecular dynamics in the overlap domain are coupled through a constrained particle dynamics. The constrained particle dynamics is constructed with a virtual damping force and a virtual added mass force. The sudden-start Couette flows with either non-slip or slip boundary condition are used to test the hybrid method. It is shown that the results obtained are quantitatively in agreement with the analytical solutions under the non-slip boundary conditions and the full MD simulations under the slip boundary conditions.

Keywords   Hybrid method · Molecular dynamic simulation · Navier–Stokes equation · Microfluidics

J. Cui · G. W. He (✉)
LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China
e-mail: hgw@lnm.imech.ac.cn

G. W. He
e-mail: guoweihe@yahoo.com

D. Qi
Department of Paper and Chemical Engineering, Western Michigan University, Kalamazoo, MI 49008, USA

1 Introduction

Micro- and nano-fluidics have attracted increasing attentions, since they have extensive applications to micro-electro-mechanical system (MEMS) that involves flows at micro- and nano-scales [1]. As the scales are decreased, the flows at micro- and nano-scales exhibit the properties very different from the flows at macroscales. The main reasons for those differences include the increasing ratio of surface to volume and the important effects of the interfaces between fluid and solid or two-phase flows [2]. Especially, in the fluid–solid interface, there may exist slip boundary conditions [3,4]. The slip boundary conditions are difficult to be treated at the level of continuum dynamics. Apparently, molecular dynamics (MD) is a powerful tool to probe the microscopic behaviors of fluids at the interfaces [5]. However, MD simulations are computationally intensive and can only study the flows over relatively short space and time scales according to the current computation capability. Therefore, it is not realistic to study micro- and nano-fluidics using a full MD simulation.

For the purpose of taking the advantages of both continuum dynamics and MD, a hybrid scheme [6] has been recently developed to solve the problems above, which combines a particle description with a continuous one. The scheme is sketched in Fig. 1. It describes the fluid as amount of particles in one domain where the MD is used, and as continuum hydrodynamics in another domain where the NS equations are used. These two solutions are coupled in the overlap domain. Thus, the boundary conditions for the NS equations, which are not explicitly available at micro- and nano-scales, can be obtained from MD simulations. The computational time in the hybrid method is expected to be much shorter than the
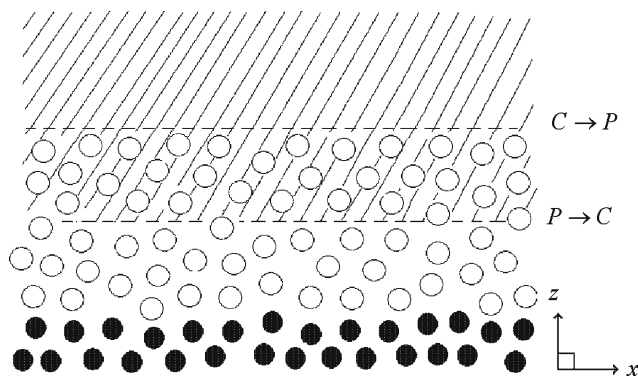
Fig. 1 A schematic diagram for the hybrid method. *Circles* indicate the particle region: *empty ones* represent the fluid and *solid ones* represent the solid substrate; *straight lines* indicate the continuum region. $C \rightarrow P$ is the upper surface of the particle region and $P \rightarrow C$ is the lower surface of the continuum region. The overlap region is in between the two surfaces

full MD computation in the flow region, since most of the computational region is solved by the NS equations. The challenge is how to couple the continuum dynamics and MD to ensure the continuity of the physical quantities, such as density, momentum, energy and their fluxes, in the overlap domain.

Several coupled models have been proposed. O'Connell and Thompson [7] developed a constrained particle dynamics for stress continuity; Hadjiconstantinou and Patera [8] presented a heterogeneous algorithm for incompressible flows; Flekkoy et al. [9] developed a flux-exchange scheme to couple particle dynamics with continuum dynamics. Recently, Nie et al. [10] developed a coupling model using a constraint force. All of these methods have made different contributions for different purposes. We have used O'Connell and Thompson's model and Nie et al.'s model to simulate a sudden-start Couette flow with isothermal Newtonian fluid. It is observed that the evolution rates of velocities are strongly dependent on an adjustable coefficient in O'Connell and Thompson's model and an imposed constraint force in Nie et al.'s model.

In present paper, we develop a coupling model in terms of a virtual damping force and a virtual added mass force in Sect. 2; The model is assessed in terms of the evolution rates of velocities in the Couette flows with the non-slip boundary conditions, and is also used to simulate the Couette flows with the slip boundary conditions in Sect. 3; The summary is given in Sect. 4.

2 Hybrid computations

In the hybrid scheme, a computation domain is decomposed into three regions: a particle region treated by

MD, a continuum region treated by the NS equations and a particle-continuum overlap region treated by a constrained particle dynamics. The constrained particle dynamics has to be constructed such that the particle representation is consistent with both continuum dynamics and MD.

In the MD region, fluid is represented by spherical particles. The particles separated by a distance r interact in terms of a shifted Lennard–Jones (LJ) potential:

$$V^{\mathrm{LJ}} = 4\epsilon \left[(\sigma/r)^{12} - (\sigma/r)^6 - (\sigma/r_c)^{12} + (\sigma/r_c)^6 \right], \quad (1)$$

where ϵ and σ are the characteristic energy and length scales, respectively. The cutoff length is set to be $r_c = 2.2\sigma$, which means that the interactions vanish when the particle separations are larger than r_c. Each particle has the mass m and the mass density is $\rho = 0.81\, m\sigma^{-3}$. The equations of motion are integrated by the Verlet scheme:

$$r_i(t + \Delta t_{\mathrm{MD}}) = 2r_i(t) - r_i(t - \Delta t_{\mathrm{MD}}) + \Delta t_{\mathrm{MD}}^2 F_i/m, \quad (2)$$

$$v_i(t) = \frac{r_i(t + \Delta t_{\mathrm{MD}}) - r_i(t - \Delta t_{\mathrm{MD}})}{2\Delta t_{\mathrm{MD}}}, \quad (3)$$

where r_i is the position of i-th particle, v_i the velocity of i-th particle and F_i the force adding to i-th particle by all other particles. The time step is $\Delta t_{\mathrm{MD}} = 0.005\tau$, in which $\tau = \sqrt{m\sigma^2/\epsilon}$ is the characteristic time of the LJ potential. These quantities will be non-dimensionalized via the parameters m, σ, τ and ϵ.

A Langevin thermostat is used to maintain a constant temperature T. This can be achieved by adding a Langevin noise and a frictional force to the equations of motion [11]

$$m\frac{\mathrm{d}^2 r_i}{\mathrm{d}t^2} = F_i - m\Gamma\frac{\mathrm{d}r_i}{\mathrm{d}t} + \eta_i, \quad (4)$$

where Γ is a friction constant that controls the rate of exchange with the thermostat, and η_i is the Gaussian random force of the zero mean and the variance being $2mk_{\mathrm{B}}T\Gamma$ (k_{B} is the Boltzmann constant). The thermostat is kept on the homogeneous plane with the rate $\Gamma = \tau^{-1}$.

In the continuum region, the dynamics of incompressible fluid is described by the NS equations

$$\nabla \boldsymbol{u} = \boldsymbol{0}, \quad (5)$$

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho\boldsymbol{u}\nabla\boldsymbol{u} = -\nabla p + \mu\nabla^2\boldsymbol{u}. \quad (6)$$

Here $\boldsymbol{u}$ is the fluid velocity, p the pressure, ρ the constant density and μ the viscosity. The NS equations are numerically solved by the explicit projection method on staggered grids [13]. Figure 2 shows the physical quantities defined on the grids on the x–z plane: the pressures
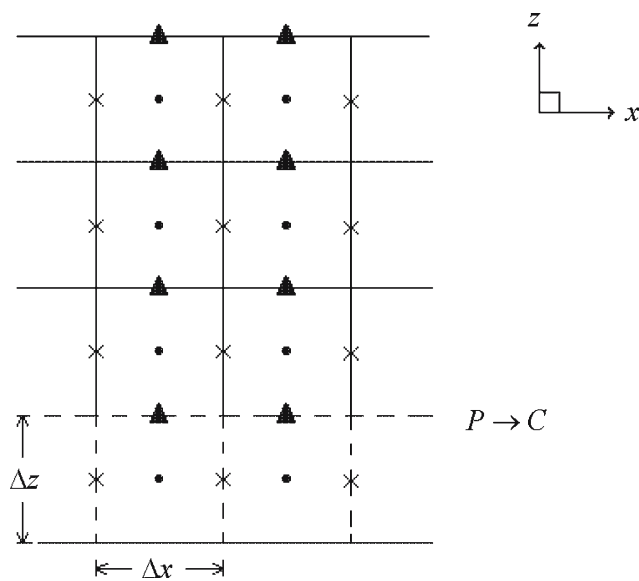
Fig. 2 A schematic diagram for the staggered grids in the continuum region. *Cross* and *triangle* indicate the x and z components of the velocities, respectively. Δx and Δz are the length of the grid in x and z directions. *Dashed lines* denotes the cells where the boundary conditions for the NS equations are needed

Fig. 3 A schematic diagram of the constrained layer. The region between $z = a$ and $z = b$ denotes the constrained layer. *Arrows* show the external forces applied to the particles in the layer

are defined at the center of the cell and the velocities defined at the middle of the cell's sides. The time step Δt_{FD} for numerical integration should be much smaller than the characteristic time of flows: $\Delta t_{FD} \ll \rho \Delta x \Delta z / \mu$.

In the overlap region, the boundary conditions for the NS equations are obtained from averaging the velocities of the particles around. The selected particles are within a volume of the size $\Delta x \times \Delta y \times \Delta z$ that is centered at the point of interest. To reduce the errors brought by MD's randomicity, we also average the quantities by several MD time steps. The constrained particle dynamics in the overlap region will be developed later in this section.

As shown in Fig. 3, in the overlap region, there exists a thin constrained layer adjacent to the interface $C \rightarrow P$. In this layer, the mass fluxes are imposed, i.e., 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 is

$$n = -A\rho u_z \Delta t_{FD}/m. \tag{7}$$

Here, A is the area of the cell whose boundary is perpendicular to the interface. If n is positive, n particles are inserted at regular intervals Δt_{FD}, and placed near the interface $C \rightarrow P$ in z direction and randomly in x and y directions. To prevent the inserted particles being too close to the previous ones, we drop out such kind of particles and repeat the process until the inserted particles have the appropriate distances to the previous ones. The initial velocities of the inserted particles are set to
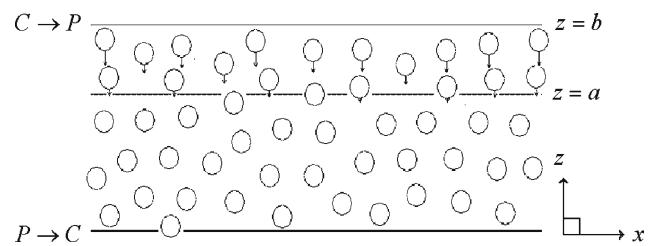
be the same as the macroscopic velocities at the cell boundary in order to ensure that the averaging velocities of particles are consistent with the flow velocities. If n is negative, n particles closest to the interface $C \rightarrow P$ are removed. At each interval Δt_{MD}, the nearest integer to n is taken.

In order to maintain momentum flux continuity, the following assumptions must be satisfied [9]

$$\sum_i F_i' = A\left(-P + 2\mu \frac{\partial u_z}{\partial z}\right), \tag{8}$$

$$\langle \boldsymbol{v} \rangle = \boldsymbol{u}, \tag{9}$$

where F_i' is an external force acting on i-th particle in the constrained layer, P the local pressure, $\langle \boldsymbol{v} \rangle$ the average velocity of particles and $\boldsymbol{u}$ the velocity from the NS equations. The right-hand side of Eq. (8) will be denoted by F in the following text. It indicates that the sum of the additional forces on the particles in the constrained layer is determined by the continuum dynamics. To prevent the particles from spreading freely away from the MD domain, we take F_i' as the following form

$$F_i' = \frac{g(z^i)}{\sum_j g(z^j)} F, \tag{10}$$

and

$$g(z^i) = \frac{1}{(b-a)-(z^i-a)} - \frac{1}{b-a} - \frac{z^i-a}{b^2}, \tag{11}$$

where $g(z^i)$ is an arbitrary weight function dependent on the position of i-th particle in z direction. The function $g(z^i)$ is chosen such that the force F_i', which is applied to the particles adjacent to the interface $C \rightarrow P$ ($z = b$), approaches $[(b-a)-(z^i-a)]^{-1}$, and the force F_i', which is applied to the particles on the surface $z = a$, is equal to zero. As a result, the particles are effectively constrained in the MD domain.

Equation (9) requires that the average velocities of particles must match the macroscopic velocities in the constrained layer. This requirement has to be extended to the whole overlap region. To achieve the matching,

we introduce a constrained particle dynamics

$$\frac{d^2 x_i}{dt^2} = \frac{F_i}{m} + \frac{c}{m}\left(u_J - \frac{1}{N_J}\sum_{k=1}^{N_J} v_k\right) + \xi, \quad (12)$$

where $F_i = -\sum_{j \neq i}\frac{\partial V^{LJ}}{\partial r_i}$ is the force from the LJ potential, N_J the total number of the particles in the J-th cell, u_J the flow velocity at the center of the J-th cell, v_k the velocity of the k-th particle in the J-th cell, c a damping coefficient and ξ a virtual force. The summation of Eq. (12) over all particles in the J-th cell yields

$$\xi = \frac{1}{N_J}\sum_{k=1}^{N_J}\frac{d^2 x_k}{dt^2} - \frac{1}{N_J}\sum_{k=1}^{N_J}\frac{F_i}{m}. \quad (13)$$

Thus, the submission of Eq. (13) into Eq. (12) gives

$$\frac{d^2 x_i}{dt^2} = \left[\frac{F_i}{m} - \frac{1}{N_J}\sum_{k=1}^{N_J}\frac{F_k}{m}\right]$$
$$+ \frac{c}{m}\left(u_J - \frac{1}{N_J}\sum_{k=1}^{N_J} v_k\right) + \frac{d}{dt}\left(\frac{1}{N_J}\sum_{k=1}^{N_J} v_k\right). \quad (14)$$

The second term on the right-hand side of Eq. (14) is an analog of the damping force due to the velocity differences between particles and flows; the third term is another analog due to the added mass force. In conformity with the properties of liquids [12], the Stokes damping coefficient $c = 3\pi\sigma\mu$ is taken into Eq. (14); and the coefficient $-\pi\sigma^3\rho/(12m)$ for the added mass force is also introduced into Eq. (14). Discretization of Eq. (14) with those coefficients yields

$$\frac{x(t + \Delta t_{MD}) - 2x(t) + x(t + \Delta t_{MD})}{\Delta t_{MD}^2}$$
$$= \frac{F_i}{m} - \frac{1}{N_J}\sum_i\frac{F_i}{m} + \frac{3\pi\mu\sigma}{m}\left(u_J - \frac{1}{N_J}\sum_i v_i\right)$$
$$- \frac{\pi\sigma^3\rho}{12m}\frac{\frac{1}{N_J}\sum_i v_i(t) - \frac{1}{N_J}\sum_i v_i(t - \Delta t_{MD})}{\Delta t_{MD}}. \quad (15)$$

This is the constrained particle dynamics in the overlap region. In the computations, we first solve the NS equations for the solution at $t + \Delta t_{FD}$, then we run the MD computation using the constrained particle dynamics Eq. (15) in the overlap domain until their velocities are matched. Meanwhile, u_J in Eq. (15) is a fixed value at each Δt_{FD}. Therefore, we do not need the extrapolations for macroscopic velocities at each Δt_{MD} from the continuum dynamics.

3 Results

The hybrid method developed in last section is used to simulate sudden-start Couette flows 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. In this section, we will consider the Couette flows with either non-slip or slip boundary conditions.

The Couette flow is the viscous fluid confined between two parallel plates, in which the top plate at $z = H = 52.1\sigma$ is moving with a velocity $U_w = \sigma/\tau$ in x direction and the bottom one at $z = 0$ is fixed, see Fig. 4. The Couette flow is simulated in the rectangle domain of $26.05\sigma \times 52.1\sigma$ in the x–z plane. A periodic boundary condition is imposed in the streamwise direction. We discretize the flow domain into the uniform grid $\Delta x \times \Delta y = 5.21\sigma \times 5.21\sigma$. The grid number is 5×10. In the hybrid method, the computation domain in $0 \leq x \leq 26.05\sigma$ and $0 \leq z \leq H$ is divided into two regions: the upper one at $z_1 \leq z \leq H$ ($z_1 = 15.63\sigma$) is the continuum region which is described by the NS equations, and the boundary condition at z_1 of the NS equations is taken from the results of MD; the lower one at $0 \leq z \leq z_2$ ($z_2 = 31.26\sigma$) 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 $z_1 \leq z \leq z_2$ is solved by the constrained particle dynamics. The overlap region is chosen large enough to guarantee the consistence of momentum between continuum and particle descriptions and small enough to save the computational time as much as possible.

In the hybrid method, the boundary condition at $z = z_2$ is given in Sect. 2 using a thin constrained layer; The boundary condition at $z = 0$ is simulated by two (111) 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 $\epsilon^{wf} = 0.6\epsilon$, 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 $(0.6\epsilon, 0.75\sigma, 4\rho)$ and $(0.2\epsilon, 0.75\sigma, 4\rho)$ yield two different slip boundary conditions [3]. Those are the benchmark test cases for validation and verification of the hybrid methods.

The overlap domain has three cells in the normal direction and the constrained layer consists of the cells nearest to the interface $C \rightarrow P$. In the molecular dynamics simulation, the temperature maintains $T = 1.1\epsilon/k_B$ and at those given T and ρ, the fluid is in a well-defined liquid phase with viscosity $\mu = 2.14\epsilon\tau\sigma^{-3}$. The viscosity is also used in the continuum region. We first run the
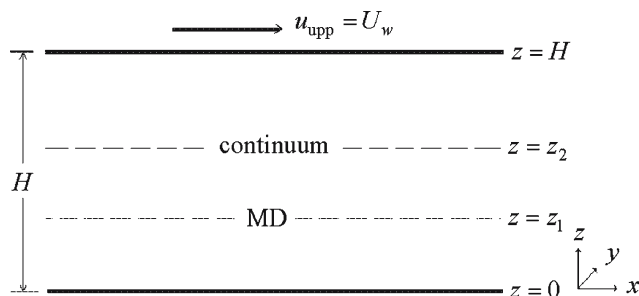
Fig. 4 A schematic diagram of the Couette flows. H denotes the distance between the two plates. $z = 0$ denotes the bottom plate, $z = z_1$ denotes the surface $P \rightarrow C$ and $z = z_2$ denotes the surface $C \rightarrow P$. U_w is the moving velocity of the top plate in the x direction
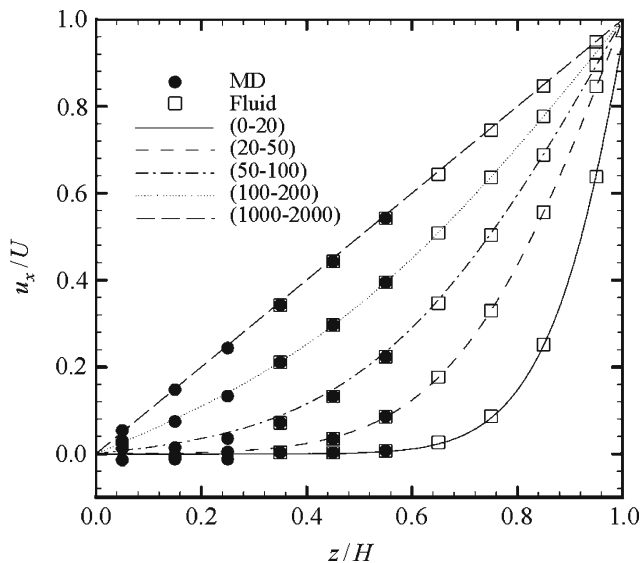

Fig. 5 Velocity profiles at different times from the hybrid method and analytical solutions of the Navier–Stokes equations. *Lines* denote the analytical solution from the Navier–Stokes equations; *empty squares* denote the result in the continuum region and *solid circles* denote the one in the particle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

simulation in the MD region for 200τ to a relative steady state from the initial positions and velocities. The hybrid simulations run for $2,000\tau$ to achieve a steady state.

Figure 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 ten independent runs. It can be seen that the results from the hybrid method follow the ones from the analytical solutions. Especially, in the overlap domain, 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.
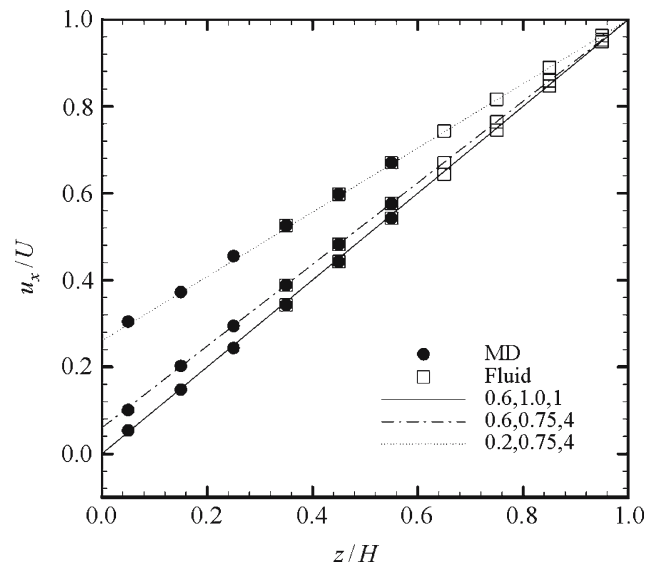

Fig. 6 Steady velocity profiles of the Couette flows under the non-slip and slip boundary conditions. The *inlet* indicates the symbols of the results obtained from the hybrid method and full MD computation

Figure 6 shows the steady solutions of the sudden-start Couette flows with two different slip boundary conditions at the bottom plate. For comparison, we also plot the velocity profile of the Couette flows with the non-slip boundary condition. The different slip velocities at the bottom plates do induce the velocity profiles of different slopes, which are in agreement with the previous predictions [3]. It is verified that the hybrid method developed here is valid for the slip boundary conditions.

4 Summary and conclusions

A hybrid method has been developed for micro- and nano-fluidics. In the present method, the constrained particle dynamics is used to couple MD and continuum dynamics in the overlap region. An important feature of the constrained particle dynamics is that a virtual damping force and a virtual added mass forces are taken into account. The method is used to simulate the sudden-start Couette flows with either non-slip or slip boundary conditions. The obtained results are in agreement with the analytical solutions and the full MD simulations. The computational efficiency of the hybrid method relative to a full MD is approximately the ratio of total volume to the portion treated by MD. In the current work, the ratio is about 2/3 and thus, about 1/3 computational time can be saved. It demonstrates the potential applications of the hybrid method to micro- and nano-fluidics, especially with complex geometry.

References

1. Squires, T.M., Quake, S.R.: Microfluidics: fluid physics at the nanoliter scale. Rev. Mod. Phys. **77**, 977–1026 (2005)
2. Gad-el-Hak, M.: Transport phenomena in microdevice. ZAMM **84**, 494–498 (2004)
3. Thompson, P.A., Troian, S.M.: A general boundary condition for liquid flow at solid surface. Nature **389**, 360–362 (1997)
4. Pit, R., Hervet, H., Leger, L.: Direct experimental evidence of slip in hexadecane. Phys. Rev. Lett. **85**, 980–983 (2000)
5. Guo, W.L., Zhu, C.Z., Yu, T.X., Woo, C.H., Zhang, B., Dai, Y.T.: Formation of sp(3) bonding in nanoindented carbon nanotubes and graphite. Phys. Rev. Lett. **93**, Art. No. 245502–5 (2004)
6. Koumoutsakos, P.: Multiscale flow simulation using particle. Ann. Rev. Fluid. Mech. **37**, 457–487 (2005)
7. O'Connell, S.T., Thompson, P.A.: Molecular dynamics-continuum hybrid computations: a tool for studying complex fluid flows. Phys. Rev. E. **52**, 5792–5795 (1995)
8. Hadjiconstaniou, N.G., Patera, A.T.: Heterogeneous and atomistic–continuum representations for dense fluid systems. Inter. J. Modern. Phys. **8**, 967–976 (2004)
9. Flekkoy, E.G., Wagner, G., Feder, G.: Hybrid model for combined particle and continuum dynamics. Europhys. Lett. **52**, 271–276 (2000)
10. Nie, X.B., Chen, S.Y., Robbins, M.O.: A continuum and molecular dynamics hybrid method for micro- and nano-fluid flow. J. Fluid. Mech. **500**, 55–64 (2004)
11. Frenkel, D., Smit, B.: Understanding Molecular Simulation-from Algorithms to Applications. Academic, New York (1996)
12. Liu, D.Y.: Fluid Dynamics of Two-phase System. Higher Education Press, Beijing (1993)
13. Tannehill, J., Anderson, D.A., Pletcher, R.H.: Computational Fluid Mechanics and Heat Transfer, 2nd edn. Taylor & Francis, New York (1997)