Journal of Computational Physics 355 (2018) 534–547

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A dissipative particle dynamics method for arbitrarily complex geometries

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ARTICLE INFO

Article history:
Received 27 December 2016
Received in revised form 30 October 2017
Accepted 13 November 2017
Available online 23 November 2017

Keywords:
Coarse-graining
Mesh-free
Complex fluid
Mesoscopic model
Arbitrary geometry

ABSTRACT

Dissipative particle dynamics (DPD) is an effective Lagrangian method for modeling complex fluids in the mesoscale regime but so far it has been limited to relatively simple geometries. Here, we formulate a local detection method for DPD involving arbitrarily shaped geometric three-dimensional domains. By introducing an indicator variable of boundary volume fraction (BVF) for each fluid particle, the boundary of arbitrary-shape objects is detected on-the-fly for the moving fluid particles using only the local particle configuration. Therefore, this approach eliminates the need of an analytical description of the boundary and geometry of objects in DPD simulations and makes it possible to load the geometry of a system directly from experimental images or computer-aided designs/drawings. More specifically, the BVF of a fluid particle is defined by the weighted summation over its neighboring particles within a cutoff distance. Wall penetration is inferred from the value of the BVF and prevented by a predictor–corrector algorithm. The no-slip boundary condition is achieved by employing effective dissipative coefficients for liquid–solid interactions. Quantitative evaluations of the new method are performed for the plane Poiseuille flow, the plane Couette flow and the Wannier flow in a cylindrical domain and compared with their corresponding analytical solutions and (high-order) spectral element solution of the Navier–Stokes equations. We verify that the proposed method yields correct no-slip boundary conditions for velocity and generates negligible fluctuations of density and temperature in the vicinity of the wall surface. Moreover, we construct a very complex 3D geometry – the "Brown Pacman" microfluidic device – to explicitly demonstrate how to construct a DPD system with complex geometry directly from loading a graphical image. Subsequently, we simulate the flow of a surfactant solution through this complex microfluidic device using the new method. Its effectiveness is demonstrated by examining the rich dynamics of surfactant micelles, which are flowing around multiple small cylinders and stenotic regions in the microfluidic device without wall penetration. In addition to stationary arbitrary-shape objects, the new method is particularly useful for problems involving moving and deformable boundaries, because it only uses local information of neighboring particles and satisfies the desired boundary conditions on-the-fly.

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https://doi.org/10.1016/j.jcp.2017.11.014
0021-9991/

1. Introduction

Despite of the sustained fast growth of computing power during the past few decades, it is still computationally prohibitive or impractical to model long time scales and large spatial scales in many applications of soft matter and biological systems with the brute-force atomistic simulations [1,2]. If only the mesoscopic properties and collective behavior are of practical interest, it may not be necessary to explicitly take into account all the details of materials at the atomic/molecular level [3]. To this end, a coarse-graining approach eliminates fast degrees of freedom and drastically simplifies the dynamics on atomistic scales, while providing a cost-effective simulation path to capturing the correct properties of complex fluids at larger spatial and temporal scales beyond the capacity of conventional atomistic simulations [4]. In recent years, with increasing attention on the research of soft matter and biophysics [5], coarse-grained (CG) modeling has become a rapidly expanding methodology especially in the simulations of polymers [6–9], colloidal suspensions [10–12], interfaces of multiphase fluids [13–15], cell dynamics [16–18], blood rheology [19–21] and biological materials [22–25].

Initially proposed by Hoogerbrugge and Koelman [26], dissipative particle dynamics (DPD) is one of the currently most popular CG methods [27–29] for performing mesoscopic simulations of complex fluids. The DPD particles are defined as coarse-grained entities [30,31], which represent clusters of molecules rather than atoms/molecules directly. In contrast to molecular dynamics (MD) method, DPD allows much larger particle size and also time steps because of the soft particle interactions. As a particle-based mesoscopic method, DPD considers N particles, whose state variables of momentum and position are governed by the Newton's equations of motion [32]. For a typical DPD particle i, its time evolution follows $\dot{\mathbf{r}}_i = \mathbf{v}_i$ and $\dot{\mathbf{p}}_i = \mathbf{F}_i = \sum_{i \neq j}(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R)$ where $\mathbf{r}_i$, $\mathbf{v}_i$, $\mathbf{p}_i$ and $\mathbf{F}_i$ denote position, velocity, momentum and force vectors, respectively. The summation for computing the total force $\mathbf{F}_i$ is carried out over all other particles within a cutoff radius r_c beyond which the forces are considered negligible. The pairwise force $\mathbf{F}_{ij}$ comprises conservative ($\mathbf{F}_{ij}^C$), dissipative ($\mathbf{F}_{ij}^D$) and random ($\mathbf{F}_{ij}^R$) forces, which are expressed as [32]

$$\begin{aligned} \mathbf{F}_{ij}^C &= a_{ij}\omega_C(r_{ij})\mathbf{e}_{ij}, \\ \mathbf{F}_{ij}^D &= -\gamma_{ij}\omega_D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij}, \\ \mathbf{F}_{ij}^R &= \sigma_{ij}\omega_R(r_{ij})\mathrm{d}\tilde{W}_{ij}\mathbf{e}_{ij}, \end{aligned} \tag{1}$$

where $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$ represents the distance between two particles i and j, $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ is the unit vector from particles j to i, and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the velocity difference; $\mathrm{d}\tilde{W}_{ij}$ is an independent increment of the Wiener process [33]. Also, γ_{ij} is the dissipative coefficient and σ_{ij} sets the strength of random force. The dissipative force and random force together act as a thermostat when the dissipative coefficient γ and the amplitudes of white noise σ satisfy the fluctuation–dissipation theorem (FDT) [33,34] requiring $\sigma^2 = 2\gamma k_B T$ and $\omega_D(r) = \omega_R^2(r)$. All these forces in Eq. (1) have the same finite interaction range r_c and their amplitudes decay according to corresponding weight functions. A common choice of the weight functions [32] is $\omega_C(r) = 1 - r/r_c$ and $\omega_D(r) = \omega_R^2(r) = (1 - r/r_c)^2$ for $r \leq r_c$ and zero for $r > r_c$.

All the three forces between DPD particles are soft and short-range interactions, which allow large time steps for the time integration of the particle-based system. The soft interactions between DPD particles, unlike the hard potentials in atomistic simulations, cannot prevent fluid particles from penetrating wall boundaries [35]. It is also unlike the top–down smoothed particle hydrodynamics (SPH) [36] or smoothed DPD (SDPD) [10] approach, where the equation of state can be tuned so that the pressure is arbitrarily strong to prevent particle penetration. As a result, for wall-bounded flow systems, DPD simulations require extra formulations [37–39] to prevent the penetration of the liquid particles into solid boundaries. Specular, Maxwellian, and bounce-back reflections [40] are common techniques used to reflect particles back into the fluid after they cross the wall surface. Therefore, for wall-bounded flows one has to mathematically predefine the position of solid wall to judge the penetration of fluid particles before a DPD simulation can be performed, which is difficult to extend for arbitrarily shaped boundaries and limits the applicability of DPD.

In the present paper, we develop a boundary method for imposing correctly the no-slip boundary condition on the solid walls with arbitrary shapes. Instead of predefining the position of the wall boundary, we make the fluid particles autonomous to detect the wall surface and to infer the wall penetration by themselves based on the local information of their neighboring particles. Hence, the geometry of solid boundary can be computed on-the-fly using local particle configurations. Therefore, it is no longer necessary to predefine the boundary geometry for DPD simulations, which makes it possible to construct DPD systems with arbitrary-shape domains directly from loading experimental images or computer-aided designs/drawings. Furthermore, since this boundary method uses local information of neighboring particles and satisfies no-slip/partial-slip boundary conditions on-the-fly, it is not only valuable for stationary arbitrary-shape boundaries but also for moving boundaries and deformable boundaries.

The remainder of this paper is organized as follows: Section 2 introduces the details of the boundary method, and also how to compute the effective dissipative coefficient for liquid–solid interactions. In Section 3, we validate the proposed boundary method by performing the Poiseuille flow, the Couette flow and the Wannier flow with comparison to analytical solutions. Moreover, an error analysis of this boundary method related to the curvature of arbitrary-shaped boundaries is provided in Appendix A. We also include a demonstration of micelles flowing through a very complex microfluidic device. Finally, we end with a brief summary and discussion in Section 4.