Journal of Computational Physics 356 (2018) 303–318

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Static and dynamic properties of smoothed dissipative particle dynamics

Davod Alizadehrad, Dmitry A. Fedosov *

Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

ARTICLE INFO

Article history:
Received 2 September 2017
Received in revised form 1 December 2017
Accepted 4 December 2017
Available online 11 December 2017

Keywords:
Mesoscopic hydrodynamic simulation
Fluid compressibility
Fluid viscosity
Freezing artifacts
Flows in complex geometries
Schmidt number

ABSTRACT

In this paper, static and dynamic properties of the smoothed dissipative particle dynamics (SDPD) method are investigated. We study the effect of method parameters on SDPD fluid properties, such as structure, speed of sound, and transport coefficients, and show that a proper choice of parameters leads to a well-behaved and accurate fluid model. In particular, the speed of sound, the radial distribution function (RDF), shear-thinning of viscosity, the mean-squared displacement ($\langle R^2 \rangle \propto t$), and the Schmidt number ($Sc \sim O(10^3) - O(10^4)$) can be controlled, such that the model exhibits a fluid-like behavior for a wide range of temperatures in simulations. Furthermore, in addition to the consideration of fluid density variations for fluid compressibility, a more challenging test of incompressibility is performed by considering the Poisson ratio and divergence of velocity field in an elongational flow. Finally, as an example of complex-fluid flow, we present the applicability and validity of the SDPD method with an appropriate choice of parameters for the simulation of cellular blood flow in irregular geometries. In conclusion, the results demonstrate that the SDPD method is able to approximate well a nearly incompressible fluid behavior, which includes hydrodynamic interactions and consistent thermal fluctuations, thereby providing, a powerful approach for simulations of complex mesoscopic systems.

1. Introduction

Numerical simulation and modeling of mesoscopic systems, ranging from the self-assembly of microorganisms in a biofilm to the flow of dense suspensions of deformable particles and macromolecules in complex environments, are challenging due to a large separation of time and length scales in such systems and the presence of complex irregular geometries and boundaries (either dynamic or static, deformable or solid). A continuum approximation for such problems is often very limited due to the loss of necessary details of suspended components and particles, such as particle deformability and shape, inter-particle forces, and thermal or intrinsic stochasticity. For instance, temperature or kinetic energy is one of the key parameters in determining phase diagrams and rheological properties of amorphous systems, such as colloidal suspensions (e.g., particles, cells, vesicles, droplets, or gas bubbles in a fluid) and driven granular matter [1–3]. Other examples are active motion and thermal fluctuations of a red blood cell (RBC) membrane [4,5] and infected RBCs in malaria [6,7]. On the other hand, mesoscopic length scales are much larger than molecular length scales, making the representation on atomistic level

* Corresponding author.
E-mail addresses: d.alizadehrad@fz-juelich.de (D. Alizadehrad), d.fedosov@fz-juelich.de (D.A. Fedosov).

https://doi.org/10.1016/j.jcp.2017.12.009
0021-9991/

impractical. Thus, there exist extensive scientific efforts for the development of efficient mesoscopic simulation techniques, which must take into account hydrodynamic interactions, complex geometries, stochastic thermal fluctuations, and realistic inter-particle forces.

Particle-based simulation methods, such as multi-particle collision dynamics (MPCD) [8–10], dissipative particle dynamics (DPD) [11–13], moving particle semi-implicit method (MPS) [14], smoothed particle hydrodynamics (SPH) [15,16] etc., are attractive for the modeling of complex fluids, because they allow a relatively simple representation of complex geometries and suspended particles. Examples include microswimmers with complex motility [17,18], flow behavior of vesicles and cells [19–21], and colloidal or polymeric suspensions [22,23]. However, despite many advantages of these methods for the simulation of complex fluids, there are still a number of critical issues, such as fluid compressibility, freezing artifacts, convergence limitations, the absence of thermal noise, and thermodynamic consistency, which prevent these methods to be widely used. For instance, the MPS and SPH methods neglect thermal fluctuations, which are crucial in many mesoscopic systems. In contrast, MPCD and DPD consistently account for thermal effects, but suffer from high fluid compressibility. The MPCD method has an ideal-gas equation of state, and consequently a low speed of sound, which is on the order of the thermal velocity. DPD simulations employ soft repulsive interactions between particles, which result in a lower compressibility than that in MPCD, but an increase of the repulsive interaction strength may quickly lead to artificial particle freezing with a non-fluidic behavior [24,25]. In particular, the compressibility problem becomes prominent in simulations of dynamic systems, such as fluid flow in complex geometries and collective motion of either active or passive colloids. One example is a local accumulation or depletion of solvent particles in DPD simulations of fluid flow through irregular geometries (see Fig. 2), which leads to an erroneous pressure and stress distribution, and consequently to anomalous fluid behavior. In order to reduce density variations in DPD simulations, Yazdani et al. [26] have modified the flow driving force obtained from a pressure field by a direct solution of the Navier–Stokes (NS) equations for the same geometry. However, this proposition is not a general solution and only appropriate for some specific cases [26]. Therefore, an incompressible enough model is often essential to guarantee acceptable fluid behavior for dynamic problems.

Another critical issue of DPD and MPCD fluid models is a relatively low Schmidt number $Sc = \nu/\mathcal{D}$ (often 2–3 orders of magnitude lower than that of a real liquid [13,27]), which is defined as a ratio of the kinematic viscosity ν and the self-diffusion coefficient $\mathcal{D}$. The Schmidt number is important for mesoscopic length scales, since it characterizes the importance of Brownian diffusion to hydrodynamic momentum transfer. For instance, simulations of DNA stretching in shear flow [28,29] have shown that a low Schmidt number leads to erroneous results. Furthermore, MPCD and DPD models do not always allow a direct connection between the model parameters and physical fluid properties [10,30]. To address drawbacks of existing methods, smoothed dissipative particle dynamics (SDPD) has recently been established [31]. This mesoscopic method combines advantages of SPH and DPD and provides a possibility of having hydrodynamic interactions, thermal fluctuations, arbitrary equation of state, thermodynamic consistency, and direct input of transport coefficients [31,32]. The original SDPD formulation [31] lacks angular momentum conservation, which might be crucial in simulations of suspensions [33–35]. The source of this problem is the existence of non-central inter-particle force contributions in the original SDPD method [31]. To restore angular momentum conservation in SDPD, a modified version [33] has been proposed, where all non-central force contributions are eliminated, making this method very similar to DPD. Recently, a more general formulation of SDPD with local and global angular momentum conservation [35] has been derived by introducing an additional particle-spin variable. A particle-spin variable has been also employed within the fluid-particle model [36].

The SDPD method has been already applied in different studies, including simulation of colloidal and polymer suspensions [37,38], flow behavior of single RBCs under physiological conditions [39], margination of leukocytes [40] and small particles [41] in microvessels. A recent study [42] has focused on equilibrium properties of the SDPD method, showing its consistency with fluctuating hydrodynamics at the mesoscale. However, in spite of growing popularity of the SDPD method, SDPD non-equilibrium properties (e.g., under flow) and their relation to involved method parameters have not been investigated systematically so far. Although SDPD can employ an arbitrary equation of state, it is not immediately obvious that a specified equation of state would lead to a well-behaved fluid model. Furthermore, the previous fluid simulations have utilized simple geometries, such as straight channels and tubes, while compressibility problems, shear-thinning property of a modeled simple fluid, and convergence failure are likely to appear in irregular geometries. Thus, the main objective of this paper is to provide a set of rigorous tests and suggestions for the SDPD method, to identify its strengths and weaknesses. As a starting point, we show that DPD and SDPD fluid models may exhibit large density variations in simulations of fluid flow through irregular channels, which result in an erroneous fluid behavior. An increase of the repulsive parameter in DPD slightly improves fluid incompressibility, but quickly leads to the appearance of freezing artifacts and strong shear-thinning of fluid viscosity with an increasing shear rate. These problems in DPD become even more severe at low temperatures. The SDPD method might show similar problems if method parameters are selected inappropriately. We investigate the effect of SDPD parameters on the radial distribution function, fluid viscosity, compressibility, and Schmidt number, and suggest how a good choice of parameters leads to a well-behaved fluid model, which is nearly incompressible, weakly sensitive to temperature changes, and remains fluid-like in contrast to a gas-like model with a low Sc number. The efficient set of parameters in SDPD allows to employ the method for simulations of fluid flow in complex geometries and various dynamic systems involving complex fluids.

The paper is organized as follows. Section 2 provides details on the SDPD method with angular momentum conservation. In Section 3, our main results, including undesired fluid density variations in complex geometries due to fluid compressibility, static and dynamic properties of DPD and SDPD fluids, SDPD fluid behavior in elongational flow, and the applicability