Journal of Computational Physics 281 (2015) 301–315

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Smoothed dissipative particle dynamics with angular momentum conservation

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ARTICLE INFO

Article history:
Received 25 April 2014
Received in revised form 15 August 2014
Accepted 9 October 2014
Available online 16 October 2014

Keywords:
Mesoscopic simulation
Smoothed particle hydrodynamics
Tank-treading vesicle
Taylor–Couette flow
Shear flow
Keller–Skalak theory

ABSTRACT

Smoothed dissipative particle dynamics (SDPD) combines two popular mesoscopic techniques, the smoothed particle hydrodynamics and dissipative particle dynamics (DPD) methods, and can be considered as an improved dissipative particle dynamics approach. Despite several advantages of the SDPD method over the conventional DPD model, the original formulation of SDPD by Español and Revenga (2003) [9], lacks angular momentum conservation, leading to unphysical results for problems where the conservation of angular momentum is essential. To overcome this limitation, we extend the SDPD method by introducing a particle spin variable such that local and global angular momentum conservation is restored. The new SDPD formulation (SDPD+a) is directly derived from the Navier–Stokes equation for fluids with spin, while thermal fluctuations are incorporated similarly to the DPD method. We test the new SDPD method and demonstrate that it properly reproduces fluid transport coefficients. Also, SDPD with angular momentum conservation is validated using two problems: (i) the Taylor–Couette flow with two immiscible fluids and (ii) a tank-treading vesicle in shear flow with a viscosity contrast between inner and outer fluids. For both problems, the new SDPD method leads to simulation predictions in agreement with the corresponding analytical theories, while the original SDPD method fails to capture properly physical characteristics of the systems due to violation of angular momentum conservation. In conclusion, the extended SDPD method with angular momentum conservation provides a new approach to tackle fluid problems such as multiphase flows and vesicle/cell suspensions, where the conservation of angular momentum is essential.

1. Introduction

Mesoscopic hydrodynamic simulations, such as the lattice Boltzmann (LB) method [1], dissipative particle dynamics (DPD) [2–4], multi-particle collision dynamics (MPC) [5,6], smoothed particle hydrodynamics (SPH) [7,8] etc., are frequently used to investigate a wide range of problems including colloidal and polymer solutions, dynamics of microswimmers, tissue growth, and flow behavior of vesicles and cells. All these examples include mesoscopic length scales (e.g., the size of suspended particles) rendering the modeling on atomistic level impossible. A continuum approximation is also not appropriate

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http://dx.doi.org/10.1016/j.jcp.2014.10.017

for such problems due to the loss of necessary mesoscopic details. Thus, large scientific efforts have been invested to derive reliable and efficient mesoscopic simulation techniques, which are able to tackle a wide range of problems.

A recently established mesoscopic method, smoothed dissipative particle dynamics (SDPD) [9], combines advantages of two popular techniques namely SPH and DPD. The SDPD method for fluid flow is directly derived using a discretization of the Navier–Stokes equation similar to SPH, while the inclusion of thermal fluctuations in SDPD is similar to that in the DPD formalism. SDPD can also be considered as an improved DPD method. Advantages of the SDPD method over conventional DPD include the possibility of using an arbitrary equation of state, direct input of transport properties, and a well-defined physical scale of discretized elements or fluid particles. In addition, it has been shown that the SDPD method produces proper scaling of thermal fluctuations for different fluid particle sizes [10]. The SDPD method has been already applied to a number of problems including simulations of different particles [11] and polymers [12] in a suspension, single red blood cells in tube flow [13], margination of leukocytes [14], and margination of different particles [15] in blood flow.

Despite the advantages of SDPD over the DPD method, the original SDPD formulation [9] does not conserve angular momentum, both locally and globally. Recent numerical simulations using the MPC method [16] have shown that angular momentum conservation is essential in some problems including Taylor–Couette flow with two immiscible fluids and vesicle tank-treading in shear flow. A violation of angular momentum conservation may lead to an asymmetric stress tensor and spurious unphysical torques, resulting in erroneous simulation results. In both DPD and SDPD methods, the system consists of a number of point particles. The particle interactions are determined by the three pairwise forces: conservative, dissipative, and random. In DPD, all forces between a pair of particles are directed along the line connecting two particle centers, which automatically leads to angular momentum conservation. However, in SDPD, dissipative and random forces possess not only a part along the inter-particle axis as in DPD, but also a component perpendicular to the inter-particle axis. This perpendicular part of dissipative and random forces destroys local and global angular momentum conservation. There exist a version of the SDPD method with angular momentum conservation [17], where the perpendicular component of dissipative and random forces has been neglected resulting in a method formulation very similar to DPD. In this method the input viscosity has to be scaled by a theoretically defined coefficient which depends on space dimension. The method has been shown to properly capture the torque on a rotating particle under shear [11] and the dynamics of two rotating discs [18]. However, it is advantageous to keep a perpendicular component of the dissipative force, since it provides much more efficient control over fluid transport properties than the component along inter-particle axis alone [19].

To derive a consistent version of SDPD with angular momentum conservation, we introduce a spin variable, such that each SDPD particle possesses an angular velocity. This idea is similar to that of the fluid particle (FPM) model [20], where every particle possesses an angular velocity; however, FPM lacks a direct connection to the discretization of the Navier–Stokes equation. Also, a spin variable has been introduced in the single-particle DPD formulation [21], where a colloidal particle can be represented by a single DPD particle with spin. Consistent SDPD formulation with angular momentum conservation is obtained by a direct discretization of the Navier–Stokes equation for a fluid with spin [22]. The resulting formulation is similar to the original SDPD method [9] with the addition of a rotational friction force which governs particle-spin interactions similar to the FPM method. First simulation tests show that the newly derived method represents properly transport properties of a simple fluid performing similar to the original SDPD method. Then, the new SDPD method is validated using several problems where angular momentum conservation plays an essential role [16]. First, the Taylor–Couette flow with two immiscible fluids is simulated showing that the extended SDPD method results in predictions in agreement with the analytical solution derived from the Navier–Stokes equation. The original SDPD method applied to this problem fails to capture correctly the corresponding flow profiles. Another fluid flow problem considered for validation of the new SDPD method is a tank-treading vesicle in shear flow, which has been described theoretically by Keller and Skalak [23]. Vesicle tank-treading in shear flow corresponds to rotational motion of a membrane around the vesicle center-of-mass, while the vesicle preserves its stationary shape with a finite inclination angle. The new SDPD formulation results in predictions of vesicle inclination angles and tank-treading frequencies for several viscosity contrasts between inner and outer fluids in agreement with the Keller–Skalak theory [23], while the SDPD method without angular momentum conservation clearly fails to capture quantitatively correct dynamics.

The paper is organized as follows. In Section 2, the new SDPD approach with conservation of local and global angular momentum is derived. In Section 3, we provide simulation results for simple SDPD fluids including measurements of fluid transport properties and simulation results for the Taylor–Couette flow with two immiscible fluids. In Section 4, a tank-treading vesicle in shear flow is investigated. Finally, we conclude in Section 5 with a brief summary.

2. SDPD with angular momentum conservation

The SDPD method proposed by Español and Revenga [9] is a mesoscopic particle-based hydrodynamic approach which has been derived from the SPH [7,24] and DPD [2,3] simulation methods. More details on the DPD method are provided in Appendix A.

In the SPH method, a field variable $\tilde{g}(\mathbf{r})$ is replaced by the convolution integral of a field $g(\mathbf{r})$ and a kernel function $W(\mathbf{r}, h)$ as,

$$\tilde{g}(\mathbf{r}) \approx \int_V g(\mathbf{r}')W(\mathbf{r}-\mathbf{r}', h)\,dV', \tag{1}$$