Smoothed dissipative particle dynamics with angular momentum conservation

Kathrin Müller\textsuperscript{a}, Dmitry A. Fedosov\textsuperscript{a,*}, Gerhard Gompper\textsuperscript{a}

\textsuperscript{a}Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

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), 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 similar 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.

Keywords: mesoscopic simulation, smoothed particle hydrodynamics,
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 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 vali-
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 Sec. 2, the new SDPD approach with conservation of local and global angular momentum is derived. In Sec. 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 Sec. 4, a tank-treading vesicle in shear flow is investigated. Finally, we conclude in Sec. 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,

\[
\tilde{g}(\mathbf{r}) \approx \int_V g(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) \, dV',
\]

where the kernel function has to be differentiable and depends on the distance \( |\mathbf{r} - \mathbf{r}'| \) and the smoothing length \( h \). In addition, the integral over \( W(\mathbf{r} - \mathbf{r}', h) \) has to be normalized and the condition \( \lim_{h \to 0} W(\mathbf{r} - \mathbf{r}', h) = \delta(\mathbf{r} - \mathbf{r}') \) needs to be satisfied. For \( W(\mathbf{r}, h) \) being the delta function, we would have \( \tilde{g}(\mathbf{r}) = g(\mathbf{r}) \).

The convolution integral is discretized using small fluid volumes (or particles) such that \( \rho(\mathbf{r}')dV' \to m_j \) with \( m_j \) being the mass and \( \rho(\mathbf{r}') \to \rho(\mathbf{r}_j) \) being the mass density of particle \( j \) at the position vector \( \mathbf{r}_j \). The discretized convolution integral is then given by

\[
\tilde{g}(\mathbf{r}_i) \approx \sum_{j=1}^{N} \frac{m_j}{\rho(\mathbf{r}_j)} g(\mathbf{r}_j) W(|\mathbf{r}_i - \mathbf{r}_j|, h),
\]
where $N$ is the number of particles (Lagrangian discretization points) within the volume $V$ characterized by the smoothing radius $h$. Furthermore, derivatives of the field variable $g(r)$ follow similar approximation strategy which is described in AppendixB. Further in the text, we will also use the notations $\rho(r_j) = \rho_j$, $g(r_j) = g_j$, and $W(|r_i - r_j|, h) = W_{ij}$.

Using the SPH formalism, the continuity equation $d\rho/dt = -\rho \nabla \cdot \mathbf{v}$ becomes (see Eq. (B.10))

$$
\frac{d\rho_i}{dt} = \sum_j m_j v_{ij} \cdot \nabla_i W_{ij},
$$

(3)

where $\nabla_i W_{ij}$ can be analytically calculated. The particle density $\rho_i$ is defined as

$$
\rho_i = \sum_j m_j W_{ij}.
$$

(4)

Hence, the density of particle $i$ can be computed using its neighboring particles located within a sphere with a radius $h$. Similarly, different terms of the Navier-Stokes (NS) equation can be discretized to obtain the equations which govern particle dynamics, see AppendixB for more details.

To extend the original SDPD formulation [9], which lacks angular momentum conservation, we introduce a spin variable for every particle $\omega_i$. In addition, each particle will also possess a moment of inertia $I_i$ analogously to the already defined particle mass. We also define a function $F(r_{ij}) = F_{ij} \geq 0$ such that $\nabla_i W_{ij} = -r_{ij} F_{ij}$. In order to obtain discretized equations for the SDPD formulation with spin, we consider the NS equation with spin [25],

$$
\rho \frac{d\mathbf{v}}{dt} = -\nabla p + (\eta + \eta_r) \nabla^2 \mathbf{v} + \left(\eta + \frac{\eta_r}{3} + \xi - \eta_r\right) \nabla \nabla \cdot \mathbf{v} + 2\eta_r \nabla \times \omega,
$$

(5)

where $p$ is the pressure, $\eta$ is the dynamic shear viscosity, $\xi$ is the bulk viscosity, $\eta_r$ is the rotational viscosity, and $\omega$ is the spin angular velocity. The introduced spin variable can be interpreted in two different ways. On the one hand, it is an approach used to recover angular momentum conservation in the SDPD formulation. On the other hand, the spin can be thought of as an effective angular velocity of a fluid volume represented by a particle. However, it should not be confused with a molecular spin. The discretization of the NS equation with spin provides a consistent model, where translational and rotational friction interactions are properly balanced unlike the FPM model which does not have a direct connection to the NS equation.

Using the rules in Eqs. (A.11-A.15) of AppendixB and the Newton’s second law
of motion $m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i$, the discretization of the NS equation (5) yields the three forces: conservative (C), dissipative (D), and rotational (R) given by

$$
\mathbf{F}_{ij}^C = \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \mathbf{F}_{ij} \mathbf{r}_{ij},
$$

$$
\mathbf{F}_{ij}^D = - \left( \frac{5\eta}{3} + 3\eta_r - \xi \right) \frac{F_{ij}}{\rho_i \rho_j} \mathbf{v}_{ij} - 5 \left( \frac{\eta}{3} + \xi - \eta_r \right) \frac{F_{ij}}{\rho_i \rho_j} \mathbf{e}_{ij} (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}),
$$

$$
\mathbf{F}_{ij}^R = -2\eta_r \frac{F_{ij}}{\rho_i \rho_j} \mathbf{r}_{ij} \times (\mathbf{\omega}_i + \mathbf{\omega}_j),
$$

where $p_i$ is the particle pressure and $\mathbf{e}_{ij} = \mathbf{r}_{ij} / |\mathbf{r}_{ij}|$. The conservative force controls locally the pressure field in the system. The dissipative force provides translational friction leading to the reduction of the velocity difference between two particles. Finally, the rotational force is also dissipative, but acts on particles’ angular velocities such that a spin of one particle leads to a change in translational and angular velocity of another particle.

The defined set of deterministic forces in Eq. (6) can be referred to as a SPH discretization with angular momentum conservation. However, the SDPD method also incorporates consistently thermal fluctuations by appending a random force to the set of forces in Eq. (6). Here, the combination of dissipative, rotational, and random forces has to satisfy the fluctuation-dissipation balance. Similar to the FPM framework [20], we define a tensor $\mathbf{T}_{ij} = A(r_{ij}) \mathbf{I} + B(r_{ij}) \mathbf{e}_{ij} \mathbf{e}_{ij}$, where $A(r)$ and $B(r)$ are some functions of inter-particle distance and $\mathbf{I}$ is the unity matrix. The dissipative and rotational forces in Eq. (6) can be written in a tensorial form as

$$
\mathbf{F}_{ij}^D = - \mathbf{T}_{ij} \cdot \mathbf{v}_{ij},
\mathbf{F}_{ij}^R = - \mathbf{T}_{ij} \cdot \left( \frac{\mathbf{r}_{ij}}{2} \times (\mathbf{\omega}_i + \mathbf{\omega}_j) \right),
$$

which implies that $\eta_r = 5\eta/3 - \xi$,

$$
A(r_{ij}) = 4 \left( \frac{5\eta}{3} - \xi \right) \frac{F_{ij}}{\rho_i \rho_j}, \quad \text{and} \quad B(r_{ij}) = 10 \left( \xi - \frac{2\eta}{3} \right) \frac{F_{ij}}{\rho_i \rho_j}.
$$

Following the general framework of the fluid particle model [20], the random force can be defined as

$$
\mathbf{\tilde{F}}_{ij} dt = \sqrt{2k_B T} \left[ A(r_{ij}) d\mathbf{\tilde{W}}^S_{ij} + \frac{B(r_{ij})}{3} \text{tr}[d\mathbf{W}_{ij}] \mathbf{I} + C(r_{ij}) d\mathbf{W}_{ij}^A \right] \cdot \mathbf{e}_{ij},
$$

where $d\mathbf{W}_{ij}$ is a matrix of independent Wiener increments, $\text{tr}[d\mathbf{W}_{ij}]$ is the trace of this matrix, $d\mathbf{W}_{ij}^S = \frac{1}{2} (d\mathbf{W}_{ij} + d\mathbf{W}_{ij}^T) - \frac{1}{2} \text{tr}[d\mathbf{W}_{ij}]$ is the traceless symmetric
part, and \( dW_{ij}^A = \frac{1}{2}(dW_{ij} - dW_{ji}) \) is the antisymmetric part. The functions \( \tilde{A}(r) \), \( \tilde{B}(r) \), and \( \tilde{C}(r) \) are related to \( A(r) \) and \( B(r) \) of the tensor \( T_{ij} \) as 
\[
A(r) = \frac{1}{2} \left( \tilde{A}(r)^2 + \tilde{C}(r)^2 \right) \quad \text{and} \quad B(r) = \frac{1}{2} \left( \tilde{A}(r)^2 - \tilde{C}(r)^2 \right) + \frac{1}{4} \left( \tilde{B}(r)^2 - A(r)^2 \right) \quad \text{[20]}
\]
To further simplify the expression in Eq. (9), we select \( \tilde{C}(r_{ij}) = 0 \) leading to 
\[
\tilde{A}(r_{ij}) = \left( 2 \left( \frac{20\eta}{3} - 4\xi \right) \frac{F_{ij}}{r_{ij}} \right)^{1/2} \quad \text{and} \quad \tilde{B}(r_{ij}) = \left( 2 \left( 17\xi - \frac{40\eta}{3} \right) \frac{F_{ij}}{r_{ij}} \right)^{1/2}.
\]
The full set of forces for the SDPD method with angular momentum conservation is finally given by 
\[
\begin{align*}
F_C &= \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) F_{ij}, \\
F_D &= -\left( \gamma_a^{ij} \left( v_{ij} + \frac{\hat{e}_{ij}}{3} (\hat{e}_{ij} \cdot v_{ij}) \right) \right) - \frac{2\gamma_b^{ij}}{3} \hat{e}_{ij} (\hat{e}_{ij} \cdot v_{ij}), \\
F_R &= -\gamma_a^{ij} \frac{r_{ij}}{2} \times (\omega_i + \omega_j), \\
\tilde{F} &= \left( \sigma_a^{ij} dW_{ij} + \sigma_b^{ij} \frac{1}{3} \text{tr}[dW_{ij}] \right) \cdot \frac{\hat{e}_{ij}}{dt},
\end{align*}
\]
where 
\[
\gamma_a^{ij} = \left( \frac{20\eta}{3} - 4\xi \right) \frac{F_{ij}}{\rho_i \rho_j}, \quad \gamma_b^{ij} = \left( 17\xi - \frac{40\eta}{3} \right) \frac{F_{ij}}{\rho_i \rho_j},
\]
and \( \sigma_a^{ij}, \sigma_b^{ij} = 2\sqrt{k_B T \gamma_a^{ij}} \). It is important to note that these equations are only valid for \( 2\eta/3 \leq \xi \leq 5\eta/3 \), such that the friction coefficients \( (\gamma_a^{ij} + 2\gamma_b^{ij})/3 \) and \( \gamma_a^{ij} \) are positive. Another simplification which can be made is the reduction to a single dissipative parameters \( \gamma_{ij} \) such that \( \xi = 20\eta/21 \) and 
\[
\gamma_a^{ij} = \gamma_b^{ij} = \gamma_{ij} = \frac{20\eta}{3} \frac{F_{ij}}{\rho_i \rho_j}, \quad \sigma_a^{ij} = \sigma_b^{ij} = \sigma_{ij} = 2\sqrt{k_B T \gamma_{ij}}.
\]
Time evolution of the position and the translational and angular velocity of a particle \( i \) follows the Newton’s second law as 
\[
\begin{align*}
\dot{r}_i &= v_i, \quad \dot{v}_i = \sum_j \frac{1}{m_j} F_{ij}, \quad \omega_i = \sum_j \frac{1}{I_j} N_{ij},
\end{align*}
\]
where \( N_{ij} \) is the torque exerted by particle \( j \) on particle \( i \) and is given by \( N_{ij} = \frac{1}{2} r_{ij} \times F_{ij} \). This leads to local and global angular momentum conservation. Equation (14) is integrated using the velocity-Verlet algorithm [26]. Finally, in
simulations we use the Lucy function

\[ W(r) = \frac{105}{16\pi h^3} \left( 1 + \frac{r}{h} \right)^3 \left( 1 - \frac{r}{h} \right)^3, \]  

(15)

as a kernel function [7], which leads to \( F(r) = \frac{315}{4\pi h^5} \left( 1 - \frac{r}{h} \right)^2 \). The equation of state for the pressure is chosen to be

\[ p = p_0 \left( \frac{\rho}{\rho_0} \right)^\alpha + b, \]

(16)

where \( \rho_0 \) is the reference density, and the parameters \( p_0, \alpha, \) and \( b \) can be freely selected. This pressure equation yields the speed of sound \( c^2 = p_0\alpha/\rho_0 \), which can be easily controlled through the above parameters resulting in a good approximation of fluid incompressibility [24, 27].

The derived SDPD method with angular momentum conservation will be referred to as SDPD+a further in text. The SDPD method without angular momentum conservation [9] will be called SDPD-a. For SDPD-a, the forces are very similar to those in Eq. (11); however, the rotational force contribution is excluded. The conservative force is kept the same, while the dissipative force assumes a coefficient \( \gamma_{ij} = 5\eta F_{ij}/(3\rho_i\rho_j) \) [9] using the formulation with a single dissipative parameter as in Eq. (13), which leads to \( \xi = 0 \).

In both simulation methods, it is important to consider how the mass and for SDPD+a the moment of inertia of a fluid particle have to be assigned. For flows with low Reynolds numbers \( Re \) (i.e., in the Stokes regime), which is the main interest of the current study, the simulation results are independent of the choice of \( m \) and \( I \). However, for high enough \( Re \), particle mass should correspond to the mass of a fluid volume described by a single particle, since in SDPD particle volume can be defined. For SDPD+a, our proposition is to define similarly the moment of inertia as that of a sphere with the same volume as a simulated particle, which agrees with the suggestion in Ref. [20]. This would also lead to the moment of inertia to be a function of the particle density.

### 3. Simulations with a simple SDPD fluid

#### 3.1. SDPD fluid properties

In comparison with the DPD method, an advantage of SDPD is that transport coefficients such as fluid viscosity can be directly specified, while in DPD they often need to be computed in a separate simulation for selected fluid parameters. Furthermore, in SDPD the volume of a fluid particle is clearly defined as
\[ V = \frac{m}{\rho}, \] which also determines a physical size of the particle \[9\]. To test the validity of SDPD discretization, we calculate fluid viscosity and particle density directly in simulations for several specified viscosities, temperatures, densities, and smoothing lengths. A reverse-Poiseuille flow setup \[28\], where the flow in two halves of a computational domain is driven in opposite directions applying the same force \( f \) per particle, is used to calculate fluid viscosity using an analytical solution of the Hagen-Poiseuille equation \[29\]. The particle density is computed on the fly by averaging \( \rho \) over all particles.

![Figure 1](image.png)

Figure 1: Fluid properties of SDPD+a (blue) and SDPD-a (red) for different temperatures and pressure gradients \( \Delta P/L \), for a channel of length \( L \). (a) Measured viscosity \( \eta \) normalized by \( \eta_0 = 50\sqrt{mE/l^2} \). (b) Particle density \( \rho \) normalized by \( \rho_0 = 3m/l^3 \). The considered energy levels are \( k_B T \in \{0.1, 0.4, 1\}E \), while \( h = 1.5l \).

We introduce the basic units for the mass, \( m \) (e.g., fluid particle mass), length, \( l \), and energy, \( E \). In the simulations, this corresponds to setting \( m = 1 \), \( l = 1 \), and \( E = 1 \). For flows with low enough \( Re \) number, results should be independent of the choice of \( m \) and \( I \). We have tested our simulations for \( \eta_0 = 25\sqrt{mE/l^2} \), \( \rho_0 = 3m/l^3 \), and the five-fold increase of particle mass and moment of inertia.

As presented in Fig. C.9, the results are hardly affected by the choice of \( I \) and \( m \).

The size of a fully-periodic simulation domain has been set to \( 20l \times 40l \times 10l \), where the flow was driven along the \( y \)-axis. Model parameters for the pressure equation \(16\) have been set to \( p_0 = 100E/l^3 \), \( b = -100E/l^3 \), and \( \alpha = 7 \). For the SDPD+a fluid, the moment of inertia of every particle has been set to \( I = 1 ml^2 \). To cover a broad range of the parameter values, we performed simulations for four different viscosities \( \eta_0 \in \{25, 50, 100, 120\} \sqrt{mE/l^2} \), three energy levels \( k_B T \in \{0.1, 0.4, 1\}E \), two densities \( \rho_0 \in \{3, 5\}m/l^3 \), and two smoothing lengths \( h \in \{1.5, 3.0\}l \). For a physical fluid with \( \rho_0 \), \( \eta_0 \), and \( k_B T \), it
is then straightforward to determine $m$, $l$, and $E$. The corresponding Reynolds numbers, defined as $Re = \rho \bar{U} W / (2 \eta)$, with $W$ being the channel width, are ranging from 0.01 to 4.3. The total number of fluid particles $N$ is equal to either 24000 or 40000 depending on the chosen density. The mean particle spacing $\Delta x = (1/n)^{1/3}$, with $n = \rho / m$ being the number density, is either $\Delta x \approx 0.7$ or $\Delta x \approx 0.6$ leading to a ratio of smoothing length and mean particle spacing of $h / \Delta x \in \{2.2, 2.6, 4.3, 5.1\}$, and an average number of neighboring particles $N_n$ of $N_n \in \{42, 70, 339, 565\}$, depending on the choice of $h$ and $\rho_0$. Figure 1(a) displays the measured viscosity $\eta$ normalized by the specified viscosity $\eta_0$ with respect to the applied pressure gradient $\Delta P / L = f \rho_0 / m$, for a channel of length $L$, and for a case of $h = 1.5 l$. For both SDPD+a and SDPD-a fluids, the measured viscosity is slightly higher than $\eta_0$ for small pressure gradients, but smaller than $\eta_0$ for high pressure gradients. This effect appears to be more pronounced for a lower temperature. The particle density measurements presented in Fig. 1(b) show a slight deviation from the specified value of $\rho_0 = 3m/l^3$. However, for both SDPD+a and SDPD-a fluids the particle density values are similar. In addition, our simulations show that the particle density does not depend on the specified viscosity, since it is governed by local fluid structure of particles within a radius $h$ which is characterized by the radial distribution function.

Figure 2 presents similar measurements of fluid viscosity and particle density for a SDPD+a fluid using different $\rho_0$ values. As the particle density is increased, the mean particle spacing is reduced and the fluid properties are better approximated resulting in a smaller variation of the measured properties from the specified values. A better result obtained for higher densities is due to a larger number of neighboring particles within the interaction radius $h$, which leads to a better approximation for discretized terms of the NS equation. These results agree well with convergence studies of SPH depending on the smoothing length and the mean particle spacing [30]. Similar trends are also observed for the SDPD-a fluid. Figure 3 illustrates fluid viscosity and particle density of a SDPD+a fluid for different smoothing lengths $h$; a SDPD-a fluid yields similar results. With increasing $h$ the measured values move closer to the specified ones and the temperature dependence practically vanishes. This effect is again due to a larger number of neighboring particles within $h$ leading to smaller discretization errors for larger $h$ values. However, computational cost may increase considerably for larger $h$, since it is proportional to $h^3$ or to the number of neighboring particles. Typically it is suggested to use about 50 – 60 neigh-
boring particles in SDPD [31]; however, slightly smaller values are also possible in simulations if small variations of fluid properties are acceptable.

Figure 2: Fluid properties of a SDPD+a fluid for different pressure gradients $\Delta P/L$, for a channel of length $L$ and particle densities $\rho_0 = 3m/l^3$ (blue) and $\rho_0 = 5m/l^3$ (purple). (a) Measured viscosity $\eta$ normalized by $\eta_0 \in \{50, 100\} \sqrt{mE/l^2}$. (b) Particle density $\rho$ normalized by $\rho_0$. Different energy levels $k_B T \in \{0.4, 1\}E$ were considered, while $h = 1.5l$.

Figure 3: Fluid properties of a SDPD+a fluid for different pressure gradients $\Delta P/L$, for a channel of length $L$ and smoothing lengths $h = 1.5l$ (blue) and $h = 3.0l$ (green). (a) Measured viscosity $\eta$ normalized by $\eta_0 \in \{50, 100\} \sqrt{mE/l^2}$. (b) Particle density $\rho$ normalized by $\rho_0 = 3m/l^3$. Different energy levels $k_B T \in \{0.4, 1\}E$ were considered.

3.2. Taylor-Couette flow of two immiscible fluids

Taylor-Couette flow usually refers to a fluid flow in the gap between two rotating cylinders as shown in Fig. 4. However, we consider a setup, where the inner cylinder is replaced by another immiscible fluid such that no mixing between the two fluids at $R_i$ can occur. A solution of the incompressible NS equation for this problem yields a linear angular velocity profile $v_\phi(r) = \Omega_0 r$ across
both immiscible fluids, where \( r \) is the radial position. Note that this solution is independent of the viscosity values of the immiscible fluids. Here, it is also assumed that the system has infinite length in the cylinder-axis direction and the angular velocity \( \Omega_o R_o \) is small enough to ensure that no Taylor-Couette instabilities occur.

Recent numerical simulations with a similar setup [16] have shown that the conservation of angular momentum is necessary to obtain correct velocity and torque profiles across immiscible fluids with different viscosities. To test our new implementation of the SDPD+a method, the Taylor-Couette flow with two immiscible fluids has been simulated. Both inner and outer fluids had the following parameters:

- \( p_0 = 100 \text{E}/l^3 \), \( b = -100 \text{E}/l^3 \), \( \alpha = 7 \), \( \rho_0 = 3 \text{m}/l^3 \), \( h = 1.5L \), and \( k_B T = 0.4E \), while the ratio of fluid viscosities was set to \( \eta_i/\eta_o = 3 \).

The computational domain was assumed to be periodic in the cylinder-axis direction, while the cylinder wall was modeled by a layer of frozen particles with a thickness \( h \) whose structure (e.g., radial distribution function) was the same as that of the fluids. To prevent mixing of the fluids and particle penetration into the wall, specular reflection of particles has been imposed at cylindrical surfaces with \( r = R_i \) and \( r = R_o \). The wall particles were rotated with a constant angular frequency \( \Omega_o \) in order to generate flow. The corresponding Reynolds number is \( Re = \rho \Omega_o R_o R_i/\eta_o \approx 0.3 \). Particle mass and inertia do not affect the simulation results, as shown in Fig. C.10 for simulations with a two-fold increase/decrease of the mass and moment of inertia. Figure 5 shows angular velocity profiles for the Taylor-Couette flow using both SDPD+a and
SDPD-a methods. The SDPD+a simulation properly captures a linear profile of angular velocity, while the SDPD-a method leads to distinct slopes within the regions of different viscosities. This example illustrates the importance of angular momentum conservation and provides a validation for the new SDPD approach.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.png}
\caption{Angular velocity $v_\phi$ profiles for the Taylor-Couette flow with two immiscible fluids using both SDPD+a and SDPD-a methods. Radial position $r$ is normalized by the cylinder radius $R_o$, while angular velocity is scaled with the cylinder angular velocity $\Omega_o R_o$. The SDPD+a method leads to a correct linear profile, while the SDPD-a method fails to do so due to violation of angular momentum conservation. The SDPD-a results for different resolution with $\rho = 10\rho_0$ and for a twice larger system size (marked as "scaled") show hardly any dependence on fluid resolution.}
\end{figure}

A resolution study shows that these results are unaffected by an increase of fluid resolution in the SDPD-a method. Simulations with different densities $\rho \in \{2, 3, 5, 10\} \rho_0$ and a larger system size have led to the same angular velocities (up to a statistical averaging error) as presented in Fig. 5. A similar result is mentioned in Ref. [11], where the measured system properties were independent on the mean particle spacing of a SPH approach without angular momentum conservation. Thus, increase of resolution in SDPD-a does not seem to resolve the problem of angular momentum conservation. Currently, the origin of this observation is not clear and requires further investigation.

4. Tank-treading of a vesicle in shear flow

Flow dynamics of soft deformable objects such as liquid droplets, lipid vesicles, red blood cells, and elastic capsules has attracted a lot of scientific interest recently due to a wide range of possible applications. For instance, a number of experiments [32–34], theoretical approaches [23, 35–37], and simulations [36, 38–42] have shown that fluid vesicles exhibit a rich dynamical behavior in shear flow.
including tank-treading (TT) and tumbling (TB) motion. The tumbling motion corresponds to vesicle rotation around its center-of-mass nearly as a rigid body. A tank-treading vesicle in shear flow shows a stationary shape with a finite inclination angle $\theta > 0$ with respect to the flow direction, while the membrane is rotating around the center-of-mass of the vesicle, see Fig. 6. The occurrence of different vesicle motion is governed by the viscosity contrast $\lambda = \eta_i/\eta_o$ between fluids inside and outside the vesicle with viscosities $\eta_i$ and $\eta_o$, respectively. A physical explanation for the TT-to-TB transition can be derived from the two components of shear flow: an elongational part which tends to stretch and align a vesicle along the $x = y$ axis with an inclination angle of $\theta = \pi/4$ and a rotational part of the flow which exerts a torque on the vesicle membrane. Increasing of viscosity contrast leads to higher shear stresses inside the vesicle opposing its TT motion, which results in an effective torque and decrease of the vesicle inclination angle. Thus, for high enough $\lambda$ a transition from TT to TB motion occurs. Keller and Skalak (KS) [23] derived a theory which predicts the TT-to-TB transition. Moreover, the KS theory is able to predict the inclination angle $\theta$ in the vesicle TT regime.

The KS theory assumes a fixed ellipsoidal shape $(r_1/a_1)^2 + (r_2/a_2)^2 + (r_3/a_3)^2 = 1$, where $r_i, i \in \{1, 2, 3\}$ are the Cartesian coordinates and $a_i$ are the semiaxes of the ellipsoid. The motion of a vesicle is derived by considering energy balance between the energy supplied by the fluid and the energy which dissipates on the membrane and inside the vesicle. This balance leads to a differential equation given by

$$\frac{d\theta}{dt} = \frac{1}{2} \dot{\gamma} (B \cos(2\theta) - 1),$$

(17)

where $\dot{\gamma}$ is the shear rate. If $B > 1$, the vesicle is in the TT regime, and hence, a steady inclination angle can be found as $\theta = 0.5 \arccos(1/B)$, where $B$ is a
function of vesicle shape and viscosity contrast given by

\[
B = f_0 \left( f_1 + \frac{1}{f_2} \left( \frac{1}{1 + f_2(\lambda - 1)} \right) \right),
\]

\[
f_0 = \frac{2}{a_1/a_2 + a_2/a_1},
\]

\[
f_1 = 0.5 (a_1/a_2 - a_2/a_1),
\]

\[
f_2 = 0.5 g(a_1^2 + a_2^2),
\]

\[
g = \int_0^{\infty} (a_1^2 + s)^{-3/2} (a_2^2 + s)^{-3/2} (a_3^2 + s)^{-1/2} ds,
\]

\[
\alpha_i = \frac{a_i}{a_1a_2a_3}.
\]

Note that the KS theory does not consider vesicle’s membrane viscosity.

4.1. Vesicle model and simulation setup

The vesicle membrane is modeled by a collection of \( N_v \) particles on an ellipsoidal surface, which are connected by \( N_s \) edges forming a triangulated network of \( N_t \) triangles. An illustration of a vesicle structure is shown in Fig. 6. The network edges can be modeled by very soft springs to approximate the absence of a shear elasticity of a vesicle membrane and to preserve the network structure. However, the use of a spring potential appears not to be necessary, if a local area constraint
for network triangles is employed maintaining the network structure. Thus, the membrane model omits any spring-like connections leading exactly to a vanishing shear elasticity of the membrane. The model incorporates local/global area and volume constraints which mimic incompressibility of the membrane and inner fluid, respectively, and are given by

\[ V_{\text{area}} = \frac{k_a (A - A_{0}^{\text{tot}})^2}{2A_{0}^{\text{tot}}} + \sum_{j=1...N_t} \frac{k_d (A_j - A_{0}^{j})^2}{2A_{0}^{j}}, \quad (19) \]

\[ V_{\text{volume}} = \frac{k_v (V - V_{0}^{\text{tot}})^2}{2V_{0}^{\text{tot}}}, \quad (20) \]

where \( k_a, k_d \) and \( k_v \) are the global area, local area, and volume constraint coefficients. The term \( A_j \) is the instantaneous area of triangle \( j \), and \( A \) and \( V \) are the total vesicle area and volume, while \( A_{0}^{j} \) is the desired area of triangle \( j \), and \( A_{0}^{\text{tot}} \) and \( V_{0}^{\text{tot}} \) are the desired total area and volume, respectively [43, 44].

The local area constraint preserves a regular network without crossing of edges (without explicit spring connections), while the values of \( A_{0}^{j} \) are set to triangular areas of an initially triangulated vesicle surface. Membrane bending resistance is implemented using the potential energy

\[ V_{\text{bending}} = \sum_{j=1...N_t} k_b (1 - \cos(\Theta_j)), \quad (21) \]

where \( k_b \) is the bending constant and \( \Theta_j \) are the instantaneous angles between two adjacent triangles having a common edge \( j \). The bending constant is related to Helfrich’s macroscopic bending rigidity \( \kappa \) [45] as \( \kappa = \sqrt{3}k_b/2 \) [43, 44]. This construction works well for fluid vesicles, which deviate in their shape not too much from a sphere, as here. For more anisotropic shapes or for large deformations, triangles can become very elongated and the discretization incorrect. In this case dynamic triangulation has to be employed [46, 47].

The simulated ellipsoidal vesicle has a prolate shape with \( a_1 > a_2 = a_3 \) and an aspect ratio of \( a_1/a_2 \approx 1.7 \). The ellipsoid is characterized by a reduced volume \( V^* = V/(4\pi R_0^3/3) \), where \( R_0 = \sqrt{A_{0}^{\text{tot}}/(4\pi)} \) is the effective vesicle radius. In simulations we employ an ellipsoidal vesicle with \( V^* \approx 0.93 \), because an ellipsoid with this reduced volume has a nearly constant shape in shear flow [36]; nearly negligible vesicle deformation in flow justifies the comparison of simulation results with the KS theory, where a vesicle assumes a constant TT path. Vesicle simulation parameters are given in Table 1. The vesicle is placed in a box of size \( L_x = 9.3R_0 \) and \( L_y = L_z = 5.6R_0 \); the box size is large.
enough to neglect potential finite-size effects as it has been shown in Ref. [36]. Periodic boundary conditions are applied in $x$ and $z$ direction, while shear flow is generated in the $x$ direction with the flow velocity $\mathbf{v} = \hat{\gamma}(y - L_y/2)e_x$ and $\hat{\gamma}$ being the shear rate. Recent numerical simulations [48, 49] have shown that the inclination angle also depends on the Reynolds number $\text{Re} = \hat{\gamma}\rho_0 R^2_0/\eta_0$. Therefore, in all simulations we have selected $\text{Re} < 0.1$ to avoid inertial effects.

Two solid walls at $y = \pm L_y/2$ with no-slip boundary conditions are modeled with frozen wall particles. In addition, fluid particles are subject to bounce-back reflection at the walls to prevent particle penetration through the walls. The fluid parameters have been chosen as $p_0 = 100E/l^3$, $b = -100E/l^3$, $\alpha = 7$, $\rho_0 = 3m/l^3$, $h = 1.5l$, and $k_B T = 0.4E$.

Coupling between vesicle membrane motion and fluid flow is performed through friction interactions between vesicle vertices and the surrounding fluid particles using the DPD dissipative and random forces (see AppendixA); this friction coupling is identical to that used for red blood cells in flow in Refs. [43, 44].

Note that for membrane-fluid coupling DPD forces are used (not SDPD) providing conservation of angular momentum automatically. To simulate two distinct fluids separated by a membrane, two different strategies are employed. The first method for fluid separation implements bounce-back reflections of fluid particles at the membrane surface; this method will be referred to as the ‘reflection’ method further in the text. Current implementation of fluid-particle reflections provides local conservation of momentum, while angular momentum is not strictly conserved at the membrane. Another method for fluid separation does not consider particle reflections, but employs tracking of fluid particles such that a type of the particle crossing the membrane can be altered; this method will be referred to as the ‘exchange’ method further below. Thus, the type of an outer-fluid particle is changed to the type of an inner-fluid particle if this particle crosses the membrane from outside to inside and vice versa. This method for fluid separation at the membrane leads to local conservation of angular momentum. Both particle types possess the same mass and moment of

<table>
<thead>
<tr>
<th>$k_d/(k_B T/R_0^2)$</th>
<th>$k_a/(k_B T/R_0^2)$</th>
<th>$k_v/(k_B T/R_0^3)$</th>
<th>$\kappa/k_B T$</th>
<th>$\hat{\gamma}\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1145</td>
<td>11450</td>
<td>12256</td>
<td>21.7</td>
<td>0.36</td>
</tr>
</tbody>
</table>

Table 1: Vesicle parameters in units of energy $k_B T$ and effective vesicle radius $R_0$. $k_d$ is the local area constraint coefficient, $k_a$ is the global area constraint coefficient, $k_v$ is the volume constraint coefficient, $\kappa$ is the bending rigidity, and $\hat{\gamma}$ is the shear rate normalized by a characteristic vesicle relaxation time $\tau = \eta_0 R_0^3/\kappa$ with $\eta_0$ being the outer fluid viscosity.
inertia and therefore, local mass and momentum are conserved. Furthermore, it has been monitored that the average density remains constant, while the fluctuations around the average are very small.

4.2. Simulation results

The inclination angle of a TT vesicle in shear flow is calculated by

$$\theta = \arctan\left(\frac{u_y}{u_x}\right),$$

(22)

where \(u = (u_x, u_y, u_z)\) is the eigenvector of the moments of inertia tensor with the smallest eigenvalue. Figure 7(a) compares inclination angles obtained from simulations with SDPD+a and SDPD-a fluids and from the KS theory for different viscosity ratios \(\lambda\). Here, the ‘exchange’ method for fluid separation at the membrane is used. The simulation results obtained with a SDPD+a fluid agree very well with the KS theory predictions, while the results using a SDPD-a fluid show a significant overestimation of the inclination angle at large \(\lambda\). The results for \(\lambda = 1\) from both SDPD+a and SDPD-a cases coincide indicating that angular momentum conservation does not affect simulation results if inner and outer fluids have the same viscosity. The deviations of the SDPD+a results from the KS theory predictions might be due to small shape fluctuations of the vesicle and/or numerical errors indicated by error bars in Fig. 7(a). Comparison of simulated inclination angles using the ‘exchange’ and ‘reflection’ methods for the separation of inner and outer fluids at the membrane is shown in Fig. 7(b). The ‘reflection’ method does not strictly conserve angular momentum at the membrane; however, the corresponding effect on \(\theta\) seems to be rather small. Use of the ‘reflection’ method leads to a slight shift of vesicle inclination angles to smaller values.

Another property of a TT vesicle in shear flow which can be compared is the TT frequency found from the KS theory as

$$\omega = \frac{0.5 \cdot \dot{\gamma} \cos(2\theta)}{f_1 + f_2(\lambda - 1)},$$

(23)

Figure 8 displays the average TT frequency \(\langle \omega \rangle\) normalized by the shear rate \(\dot{\gamma}\) and obtained from simulations with SDPD+a and SDPD-a fluids and from the KS theory for different viscosity ratios \(\lambda\). The SDPD+a predictions for \(\langle \omega \rangle\) are close to the theoretical predictions for all simulated viscosity ratios. Again, the small deviations of the SDPD+a results from the KS theory predictions might be due to vesicle shape fluctuations and/or numerical errors. However,
simulations with a SDPD-a fluid clearly fail to provide correct predictions in comparison with the theoretical values. As expected, the values of TT frequency are underestimated for the SDPD-a case, which is associated with the overestimation of inclination angles in Fig. 7. In case of the SDPD-a fluid, the presence of two different viscosities leads to an asymmetric stress tensor \[16\] adding a stress contribution which suppresses TT frequency and results in an increased inclination angle. In case of \( \lambda = 1 \), the stress tensor is symmetric even for the SDPD-a fluid leading to correct predictions of vesicle dynamics in shear flow.

Figure 7: (a) Comparison of inclination angles \( \theta \) of a TT vesicle in shear flow obtained from SDPD+a (blue) and SDPD-a (red) simulations and from the KS theory (black) for different viscosity ratios \( \lambda \). The ‘exchange’ method for fluid separation is employed. (b) Comparison of the ‘exchange’ and ‘reflection’ methods for the separation of inner and outer fluids at the membrane surface for different \( \lambda \) values. The ‘reflection’ method does not strictly conserve angular momentum at the membrane.

Figure 8: Comparison of the average TT frequency \( \langle \omega \rangle \) normalized by the shear rate \( \dot{\gamma} \) and obtained from SDPD+a (blue) and SDPD-a (red) simulations and from the KS theory (black) for different viscosity ratios \( \lambda \). The ‘exchange’ method for fluid separation is employed.
5. Summary

We presented an extension of the original SDPD method [9], which satisfies local and global angular momentum conservation. In the new method (SDPD+a), each particle possesses an angular velocity, and its rotational contribution has been derived from the NS equation with spin following the SPH formalism. This leads to a spin variable similar to the FPM model [20]. Thermal fluctuations in SDPD+a have been also included similar to those in FPM [20] and in SDPD without angular momentum conservation (SDPD-a) [9]. Fluid properties measured directly in simulations support the correctness of the SDPD+a derivation and implementation, since measured values of fluid viscosity and particle density are very close to the specified ones. Furthermore, simulations of Taylor-Couette flow with two immiscible fluids show that SDPD+a leads to correct predictions of flow profiles in agreement with analytical results, while SDPD-a fails to capture properly flow characteristics due to violation of angular momentum conservation. Finally, simulations of vesicle dynamics in shear flow reveal that angular momentum conservation is essential to obtain correct results for the inclination angle and the rotational frequency of a tank-treading vesicle if there exists a viscosity contrast $\lambda$ between inner and outer fluids. For $\lambda \neq 1$ the SDPD+a method predicts vesicle characteristics in agreement with the Keller-Skalak theory for a vesicle in shear flow, while SDPD-a overestimates the inclination angle and underestimates the TT frequency. In conclusion, the new SDPD method with angular momentum conservation is able to correctly model flows where angular momentum conservation is necessary.

Acknowledgments

This work has been supported by the DFG Research Unit FOR 1543 SHENC – Shear Flow Regulation in Hemostasis. Dmitry A. Fedosov acknowledges funding by the Alexander von Humboldt Foundation. Kathrin Müller acknowledges support by the International Helmholtz Research School of Biophysics and Soft Matter (IHRS BioSoft). We also gratefully acknowledge a CPU time grant by the Jülich Supercomputing Center.

Appendix A. Dissipative particle dynamics

The DPD method [2, 3] is a mesoscopic particle simulation technique, where each particle represents a molecular cluster rather than an individual atom, and
can be thought of as a soft lump of fluid. The conservative force $F^C$ in DPD controls fluid compressibility, while the pair of dissipative $F^D$ and random forces $F^R$ defines a local thermostat in order to keep a DPD system at an equilibrium temperature. The DPD forces are local and act only within a selected cutoff radius $r_c$. The conservative force is typically defined as

$$F_{ij}^C = \hat{e}_{ij} a_{ij} \begin{cases} a_{ij}(1 - r_{ij}/r_c), & \text{for } r_{ij} \leq r_c, \\ 0, & \text{for } r_{ij} > r_c, \end{cases}$$

(A.1)

where $a_{ij}$ is the repulsion coefficient between particles $i$ and $j$, $\hat{e}_{ij} = r_{ij}/r_{ij}$, and $r_{ij} = |r_i - r_j|$. The dissipative force defined as

$$F_{ij}^D = -\gamma \omega^D(r_{ij})(v_{ij} \cdot \hat{e}_{ij})\hat{e}_{ij}$$

(A.2)

reduces the velocity difference $v_{ij} = v_i - v_j$ between two particles, and hence, provides friction in a simulated system. Here, $\omega^D(r_{ij})$ is a weight function and $\gamma$ is the dissipative force coefficient. The random force in DPD is given by

$$F_{ij}^R = \sigma \omega^R(r_{ij}) \xi_{ij} dt^{-1/2} \hat{e}_{ij},$$

(A.3)

$\omega^R(r_{ij})$ is the weight function, $\sigma$ is the random force coefficient, and $dt$ is the timestep. A random number $\xi_{ij}$ has to be symmetric ($\xi_{ij} = \xi_{ji}$) with zero mean ($\langle \xi \rangle = 0$) and unit variance; different random numbers have been used in DPD including Gaussian and uniform distributions.

To satisfy the fluctuation-dissipation balance, the pair of dissipative and random forces has to fulfill the conditions [3]

$$\omega^D(r_{ij}) = (\omega^R(r_{ij}))^2, \quad \sigma = \sqrt{2k_B T \gamma}.$$  

(A.4)

In general, the weight functions can be arbitrarily chosen; however a typical choice is

$$\omega^D(r_{ij}) = \begin{cases} (1 - r_{ij}/r_c)^k, & \text{for } r_{ij} \leq r_c, \\ 0, & \text{for } r_{ij} > r_c, \end{cases}$$

(A.5)

where the exponent $k = 1$ was used in the original DPD method [4]. Other values of $k$ (e.g. 0.25) have been also employed in order to increase the viscosity of a DPD fluid [50, 51]. The equation of state of a DPD fluid [4] and the
corresponding speed of sound $c_s$ are given by

$$p = k_B T + \alpha a \rho^2, \quad (A.6)$$

$$c_s^2 = \frac{\partial p}{\partial \rho} = 2\alpha a \rho, \quad (A.7)$$

where $a$ is the repulsive coefficient. Thus, in DPD the speed of sound can be controlled by changing the repulsive coefficient and/or fluid density. A significant increase of $a$ may affect the timestep and lead to freezing artifacts [3], while an increase in particle density affects considerably the computational cost.

**Appendix B. Calculation of derivatives**

We summarize the calculation of derivatives of field variables similar to those in SPH [24]. Using Eq. (2), the first derivative of a field $g$ can be approximated as

$$\frac{\partial \tilde{g}}{\partial x} = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \frac{\partial W_{ij}}{\partial x_i}, \quad (B.1)$$

where the notations are identical to those in the main text. A disadvantage of this approximation is that the derivative does not vanish for $g$ being a constant function. Therefore, a better approximation is given by

$$\frac{\partial \tilde{g}}{\partial x} = \frac{1}{\phi} \left( \frac{\partial (\tilde{g} \phi)}{\partial x} - \tilde{g} \frac{\partial \phi}{\partial x} \right), \quad (B.2)$$

where $\phi$ must be a differentiable function. Following Eq. (B.1), we then obtain

$$\frac{\partial \tilde{g}}{\partial x} = \frac{1}{\phi_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j} \phi_j (g_j - g_i) \frac{\partial W_{ij}}{\partial x_i}. \quad (B.3)$$

When $\phi = 1$, Eq. (B.3) reduces to

$$\frac{\partial \tilde{g}}{\partial x} \approx \sum_{j} \frac{m_j}{\rho_j} g_{ji} \frac{\partial W_{ij}}{\partial x_i}. \quad (B.4)$$

where $g_{ji} = g_j - g_i$. In Eq. (B.3), $\phi = \rho$ can be also selected, yielding an approximation for the first derivative as

$$\frac{\partial \tilde{g}}{\partial x} \approx \frac{1}{\rho_i} \sum_{j} m_j g_{ji} \frac{\partial W_{ij}}{\partial x_i}. \quad (B.5)$$
The choice for different discretizations ($\phi = 1$ or $\phi = \rho$) may depend on a problem of interest. For instance, when different interacting fluids with large density ratios are considered, it has been shown that the approximation in Eq. (B.3) with $\phi = 1$ is more accurate than that with $\phi = \rho$, because $\rho$ in Eq. (B.4) is included directly inside the sum [24, 52]. Furthermore, if only a single fluid is employed, an approximation $\phi_i \approx \rho_j$ can be used making the above choices for $\phi$ equivalent.

There exists another definition for the first derivative,

$$
\frac{\partial \tilde{g}}{\partial x} = \phi \left( \frac{\partial}{\partial x} \left( \frac{\tilde{g}}{\phi} \right) + \frac{\tilde{g}}{\phi^2} \frac{\partial \phi}{\partial x} \right).
$$

Following the SPH formalism [24] we obtain

$$
\frac{\partial \tilde{g}}{\partial x} \approx \phi_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( \frac{g_j}{\phi_j^2} + \frac{g_i}{\phi_i} \phi_j \right) \frac{\partial W_{ij}}{\partial x_i}.
$$

As a result, a choice of $\phi = 1$ here leads to

$$
\frac{\partial \tilde{g}}{\partial x} \approx \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( g_j + g_i \right) \frac{\partial W_{ij}}{\partial x_i},
$$

while for $\phi \approx \rho$ Eq. (B.7) becomes

$$
\frac{\partial \tilde{g}}{\partial x} \approx \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( g_j + g_i \rho_j \right) \frac{\partial W_{ij}}{\partial x_i}.
$$

A set of equations above defines different approximations of first derivatives, which can be used to derive discretizations of other differential operators in the NS equation. For instance, using Eq. (B.5) the gradient of $g(r)$ can be approximated as

$$
\nabla \tilde{g} \approx -\frac{1}{\rho_i} \sum_j m_j g_{ij} \nabla_i W_{ij},
$$

where $g_{ij} = g_i - g_j$. Similarly, the divergence and the curl of a vector field $\tilde{G}(r)$ are discretized as

$$
\nabla_i \cdot \tilde{G}_i \approx -\frac{1}{\rho_i} \sum_j m_j G_{ij} \cdot \nabla_i W_{ij},
$$

$$
\nabla_i \times \tilde{G}_i \approx -\rho_i \sum_j \frac{m_j}{\rho_i \rho_j} (G_j + G_i) \times \nabla_i W_{ij}.
$$
The second derivatives are then given by
\[
\nabla_i \left( \nabla_i \cdot \tilde{\mathbf{G}}_i \right) \approx - \sum_j m_j \frac{F_{ij}}{\rho_i \rho_j} \left( 5 \hat{e}_{ij} (\hat{e}_{ij} \cdot \mathbf{G}_{ij}) - \mathbf{G}_{ij} \right) \quad (B.13)
\]
and
\[
\nabla^2_i \tilde{g}_i \approx -2 \sum_j m_j \frac{F_{ij}}{\rho_i \rho_j} g_{ij}, \quad (B.14)
\]
where \( \hat{e}_{ij} = \mathbf{r}_{ij}/r_{ij} \) is the unity vector along the separation direction of particles \( i \) and \( j \) \[9\].

The curl of a vector field \( \mathbf{G} \) can be approximated as
\[
\nabla_i \times \tilde{\mathbf{G}}_i \approx \phi_i \sum_j m_j \frac{\rho_j}{\rho_j} \nabla_i W(r_{ij}) \times \left( \frac{\mathbf{G}_j}{\phi_j} + \frac{\phi_j \mathbf{G}_i}{\phi_i} \right), \quad (B.15)
\]
where a selection of \( \phi = 1 \) leads to
\[
\nabla_i \times \tilde{\mathbf{G}}_i \approx \sum_j m_j \frac{\rho_j}{\rho_j} \nabla_i W(r_{ij}) \times (\mathbf{G}_j + \mathbf{G}_i), \quad (B.16)
\]
while \( \phi = \rho \) results in
\[
\nabla_i \times \tilde{\mathbf{G}}_i \approx \rho_i \sum_j m_j \frac{\rho_j}{\rho_j} \nabla_i W(r_{ij}) \times \left( \frac{\mathbf{G}_j}{\rho_j^2} + \frac{\mathbf{G}_i}{\rho_i^2} \right). \quad (B.17)
\]

Appendix C. Verification of mass and inertia independence of simulation results

A number of simulations were performed to verify that simulation results are independent of the choice for particle mass and moment of inertia for low enough \( Re \) numbers. Figure C.9 illustrates that the effect of both mass and moment of inertia on the measured viscosity can be neglected for the studied range of flow \( Re \) numbers, while Fig. C.10 presents a similar test for the Taylor-Couette flow using both SDPD-a and SDPD+a methods.
Figure C.9: Measured viscosity $\eta$, scaled by $\eta_0 = 25\sqrt{mE/l^2}$ depending on the pressure gradient $\Delta P/L$, with $L$ being the channel length for different mass and moment of inertia values. The density is $\rho_0 = 3m/l^3$. Although both, mass and moment of inertia, are varied, the measured values of $\eta$ are hardly affected.

Figure C.10: Angular velocity $v_\phi$ profiles for the Taylor-Couette flow with two immiscible fluids using both SDPD-a (a) and SDPD+a (b) methods for different mass $m$ and moment of inertia $I$. The radial position $r$ is normalized by the cylinder radius $R_o$, while the angular velocity is scaled with the cylinder angular velocity $\Omega_o R_o$. For all masses and moments of inertia the same results are obtained.

References


