Direct simulations of particle suspensions in a viscoelastic fluid in sliding bi-periodic frames

Wook Ryol Hwang, Martien A. Hulsen*, Han E.H. Meijer

Materials Technology, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

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Abstract

We present a new finite element scheme for direct simulation of inertialess particle suspensions in simple shear flows of Oldroyd-B fluids. The sliding bi-periodic frame concept of Lees & Edwards [J. Phys. C 5 (1972) 1921] has been combined with the DEVSS/DG finite element scheme, by introducing constraint equations along the domain boundary. The force-free, torque-free rigid body motion of a particle is described by the rigid-ring problem and implemented by Lagrangian multipliers only on the particle boundary, which allows general treatments for boundary-crossing particles. In our formulation, the bulk stress is obtained by simple boundary integrals of Lagrangian multipliers along the domain and particles. We discuss the bulk rheology of suspensions as well as the micro-structural developments through the numerical examples of single-, two- and many-particle problems, which represent a large number of such systems in simple shear flow. We report the steady bulk viscosity and the first normal stress coefficient, from very dilute to highly concentrated systems. The results show shear-thickening behavior for both properties and the common experimental observation of the scaling of the first normal stress to the shear stress has been reproduced. Unlike Newtonian systems, two particles in an Oldroyd-B fluid result in kissing-tumbling-tumbling phenomena: they keep rotating around each other, when they are closely located. Many-particle problems reveal the occurrence of strong elongational flows between separating particles.

1. Introduction

In this paper, we present a new direct simulation technique for non-Brownian hard particle suspensions formulated with a viscoelastic (Oldroyd-B) fluid under simple shear flow in a well-defined bi-periodic domain. Through several example problems, we discuss bulk rheological properties as well as micro-structural developments due to complicated hydrodynamic interactions in such a system.

This work is an extension of our previous study [1] for suspensions in a Newtonian fluid, which used a fictitious domain method, similar to the distributed Lagrangian multipliers (DLM) method of Glowinski et al. [2], in that a fixed regular mesh is used for the entire computation and that hydrodynamic interaction is treated implicitly via a combined weak formulation. (The combined weak formulation was first implemented by Hu [3] using the arbitrary Lagrangian–Eulerian technique.) However, we combined the fictitious domain method with a well-defined bi-periodic domain concept, the Lees–Edwards boundary condition (LEbc) for the simple shear flow [4], which could transform a suspension consisting of a large number of particles into a particulate flow problem in a unit cell, diminishing finite size effect of the computational domain. Our previous work has two distinct features:

(1) Sliding bi-periodic constraints: The sliding bi-periodic domain concept of the LEbc for discrete particles has been extended to continuous fields and combined with the velocity-pressure formulation of the fictitious-domain/finite-element method by introducing the constraint equations;

(2) A rigid-ring description of particles: Inertialess particles are described by their boundary only, eliminating domain discretization of particles, which allows easy treatments of boundary-crossing particles.
This scheme has been verified to give accurate solutions (particle velocity, fluid velocity, pressure and even velocity-gradient distributions) with suitable choice of the spatial discretization. In addition, a general expression of the bulk stress was derived, which involves only boundary integrals of the Lagrangian multipliers on the domain boundary and on the boundary of particles crossing the domain boundary.

In the present paper, we consider the suspensions formulated with a viscoelastic (Oldroyd-B) fluid. To combine the viscoelasticity with our existing scheme, we employ a mixed finite-element formulation developed by Guénette and Fortin [5], the Discrete Elastic-Viscous Stress Splitting (DEVSS) method, which appears to provide one of the most robust formulations currently available. The discontinuous Galerkin (DG) formulation of Fortin and Fortin [6] will be used for the discretization of the constitutive equation. The use of DG is particularly suited in this work not only because of its minimal coupling between elements, avoiding a large number of coupled equations, but also from the inherent discontinuous nature of the fictitious domain method. The viscoelastic stress is discontinuous across the particle boundary.

Concentrating on the simulations of circular disk particles in 2-D, we discuss the bulk rheological properties and micro-structural developments in flowing suspensions formulated with an Oldroyd-B fluid, through numerical examples of the single-, two- and many-particle problems. Because of the bi-periodicity in the computational domain, a system possessing a few particles in a single domain represents a problem with a large number of particles in an unbounded domain. Using the single-particle problem, we report the steady bulk viscosity and the first normal stress difference coefficient as a function of the Weissenberg number and the solid area fraction. The results show shear-thickening behaviors for both properties. Interestingly, our direct simulations in 2-D reproduce the common experimental observation that the first normal stress difference in a filled viscoelastic fluid is a power-law function of the imposed shear stress such that \( N_1 \approx \tau^n \) with a power-law exponent \( n \) which is determined by the unfilled viscoelastic fluid [8–10]. (For the Oldroyd-B fluid, the exponent \( n \) becomes 2.) From the two-particle problems, we report clustering of particles, when they are closely located. It results in kissing-tumbling-tumbling phenomena of the two particles: they keep rotating around each other. This tendency becomes stronger with increasing fluid elasticity. Through the many-particle problems, we discuss developments of strong elongational flows between separating particles and the resultant non-uniformity and anisotropy in the micro-structures will be highlighted.

The paper is organized as follows. First, we state the governing sets of equations for the fluid, the particles and the hydrodynamic interactions in the strong form. Next, we present the combined weak formulation of the whole system and discuss details of the numerical implementation methods. Subsequently, we use three sets of example problems – the single, two and many particles in a sliding bi-periodic domain – to demonstrate the feasibility of our scheme and, through these examples, we discuss the rheological properties and microstructural developments in suspensions formulated with the viscoelastic fluid.

2. Modeling

2.1. Problem definition

In this paper, we consider suspensions of freely suspended rigid particles in an Oldroyd-B fluid under simple shear flow. We restrict ourselves to 2-D systems composed of circular disk-like particles, neglecting inertia for both the fluid and the particles. By combining the bi-periodic domain concept of Lees and Edwards [4], such a suspension problem can be treated as a particulate flow problem in a unit cell or frame. In this way, we can diminish finite size effects of the computational domain, eliminating complex wall interactions, and solve the problem at a reasonable computational cost.

Fig. 1 shows the sliding bi-periodic frames with a possible particle configuration in a single frame. As time goes on, each frame translates at its own average velocity of the flow inside the frame and thereby rows of the frames slide relatively to one another by the amount \( \Delta \), which is determined by the given shear rate \( \dot{\gamma} \), the elapsed time \( t \), and the height of the frame \( H \):\n
\[
\Delta = \dot{\gamma} H t. \quad (1)
\]

The sliding velocity of the frame is determined by the given shear rate and a representative vertical position of the frame based on an arbitrary global reference. Since it is an inertial frame of reference, only the relative velocity inside the frame is important. In addition, the sliding frame is bi-periodic: the left and right boundaries satisfy the usual periodic condition and the upper and lower boundaries are subject to the time-dependent sliding periodicity described by Eq. (1). Therefore the motion of the rigid particles as well as of the fluid particles is subject to the time-dependent coupling between the upper and lower boundaries, in addition to the usual periodic condition in the horizontal direction. For details of the sliding bi-periodic frame, refer to Hwang et al. [1].

A sliding bi-periodic frame, denoted by \( \Omega \), is the computational domain of this work (Fig. 1). The four boundaries of the domain are denoted by \( \Gamma_i (i = 1, 2, 3, 4) \) and the symbol \( \Gamma \) will be used for \( \bigcup_{i=1}^{4} \Gamma_i \). The Cartesian \( x \) and \( y \) coordinates are selected as parallel and normal to the shear flow direction, respectively. Particles are denoted by \( P_i(t) \) \((i = 1, \ldots, N)\) and \( N \) is the number of particles in a single frame. We use a symbol \( P(t) \) for \( \bigcup_{i=1}^{N} P_i(t) \), a collective region occupied by particles at a certain time \( t \). For a particle \( P_i \), \( (x_i, y_i) \) are used for the coordinates of the particle center, the translational velocity, the angular velocity and the angular rotation.
tion, respectively; and $k$ is the unit vector in the direction normal to the plane.

2.2. Governing equations

We present the governing equation sets in the strong form for suspensions of 2-D disk-like circular particles in an Oldroyd-B fluid in a sliding bi-periodic frame, neglecting inertia for both the fluid and the particles.

2.2.1. Fluid domain

The set of equations for the fluid domain is given by

\[ \nabla \cdot \sigma = 0, \quad \text{in } \Omega(P(t)), \]  
\[ \nabla \cdot u = 0, \quad \text{in } \Omega(P(t)), \]  
\[ \sigma = -pI + 2\eta \dot{D} + \tau, \quad \text{in } \Omega(P(t)), \]  
\[ \lambda \tau = \tau_p - 2\eta \dot{D} = 0, \quad \text{in } \Omega(P(t)), \]  
\[ u = U_i + \omega_s \times (x - X_i), \quad \text{on } \partial \Omega, i = 1, \ldots, N. \]  

Eqs. (2)-(6) are equations for the momentum balance, the continuity, the constitutive relation of the Oldroyd-B fluid in a sliding bi-periodic frame, neglecting inertia for both the fluid and the particles.

In the weak formulation, the kinematic constraints are more complicated because of the time-dependent coupling between $\Gamma_1$ and $\Gamma_3$ as described in Eq. (1) . Below are the kinematic condition for the continuity, the force balance and the continuity of the polymer stress, respectively.

\[ u(x, H; t) = u([(x - yH)^x, 0, t) + f], \quad x \in [0, L], \]  
\[ t(x, H; t) = t([(x - yH)^x, 0, t), \quad x \in [0, L], \]  
\[ \tau_p(x, H; t) = \tau_p([(x - yH)^x, 0, t), \quad x \in [0, L], \]  

where $f = (yH, 0)$ and $[,]^x$ denotes the modular function of $L$. (For example, $[1.7L]^x = 0.7L$ and $[-1.7L]^x = 0.3L$.)

Eqs. (8)-(13) completes the governing equations with Eqs. (2)-(7) for the fluid domain in the strong form.

In the weak formulation, the kinematic constraints (Eqs. (8) and (11)) are usually combined with Lagrangian multipliers and then the associated force balances (Eqs. (9) and (12)) are satisfied implicitly through the multipliers. In this regard, we will use the kinematic equations...
(Eqs. (8) and (11)) in derivation of the weak form and we call the two equations the sliding bi-periodic constraints. The continuity conditions for $\tau_p$ (Eqs. (10) and (13)) will be treated separately through the jump convection term in the discontinuous Galerkin (DG) formulation, which will be discussed in Section 3.1.

2.2.2. Particle domain

As we did in [1] for particles in a Newtonian fluid, we again use the rigid-ring description for the particle domain in the viscoelastic fluid, which holds whenever inertia is negligible. With this description, a particle is considered as a rigid ring, which is filled with the same fluid as in the fluid domain, and the rigid-body motion is imposed only on the particle boundary. The idea is similar to the original immersed boundary method of Peskin [12] in which the equations for the fluid velocity is solved for both inside and outside of the moving boundary of zero mass. This description needs discretization only along the particle boundary so that it gives significant reduction in memory and it is easier to implement, especially for boundary-crossing particles, compared with methods using domain discretization [2,13–15].

In addition, the traction force on the particle boundary can be obtained as a part of the solution, when the constraint equation of the rigid-body motion is combined with Lagrangian multipliers [1].

The particle $P_i$ ($i = 1, \ldots, N$) in an Oldroyd-B fluid is described by the following set of equations:

$$\nabla \cdot \sigma = 0, \quad \text{in} \quad P_i(t),$$

$$\nabla u = 0, \quad \text{in} \quad P_i(t),$$

$$\sigma = -pI + 2\eta \dot{D} + \tau_p, \quad \text{in} \quad P_i(t),$$

$$\lambda \dot{\tau}_p + \tau_p - 2\eta_p \dot{D} = 0, \quad \text{in} \quad P_i(t),$$

$$u = U_i + \omega \times (x - X_i) \quad \text{on} \quad \partial P_i(t).$$

Eqs. (14)-(18) are equations for the momentum balance, the continuity, the constitutive relation (Oldroyd-B) and the boundary condition, respectively, which are exactly the same as the fluid domain equations as in Eqs. (2)-(6). The initial condition for the polymer stress is again the stress-free state, as it should be inside the rigid-ring, i.e.

$$\tau_{p,0} = 0, \quad \text{in} \quad P_i(t).$$

We do not need an inflow condition for the polymer stress $\tau_p$, since there is no net convection of material particles across the particle boundary. The solution of the rigid-ring problem (Eqs. (14)-(19)) inside the particle appears to be the rigid-body motion imposed on the particle boundary:

$$u = U_i + \omega \times (x - X_i) \quad \text{in} \quad P_i(t).$$

Due to the rigid-body motion, the polymer stress inside the rigid-ring remains zero. Finally, the motion of the particle center is given by the following advection equations:

$$\frac{dX_i}{dt} = U_i, \quad X_{|t=0} = X_{ib}.$$

Note that Eq. (22) is completely decoupled from the other equations.

2.2.3. Hydrodynamic interaction

In order to determine the unknown rigid body motions $(U_i, \omega_i)$ of the particles, one needs balance equations for drag forces and torques on particle boundaries. In the absence of inertia and external forces or torques, particles are force-free and torque-free:

$$F_i = \int_{\partial P_i(t)} \sigma \cdot n \, ds = 0,$$

$$T_i = \int_{\partial P_i(t)} (x - X_i) \times (\sigma \cdot n) \, ds = 0,$$

where $T_i = T_i k$ and $n$ is a normal vector on $\partial P_i$ pointing out of the particle.

We did not use an artificial particle-particle collision scheme [2,13–15], because the particle overlap could be avoided for the multiple-particle problems we studied in this paper by taking a relatively small time-step and a sufficiently refined particle boundary discretization.

2.3. Boundary-crossing particles

When a particle crosses the domain boundary, the particle or parts of the particle, which are present outside the computational domain, need to be relocated into the domain. The relocation possibly involves the change of the translational velocity of the particle, since the upper (lower) sliding frame moves faster (slower) than the frame of computation by the amount of the velocity difference $\gamma H$. We discussed the treatment of such a situation in details with the sliding bi-periodic domain in Hwang et al. [1]. Here we briefly summarize the method for completeness of the paper.

The relocation can be made in two consecutive steps: relocation of the particle center and of the particle boundary. Both of them can be expressed in a single equation. Consider two sets of the coordinates: the unprimed set for the original coordinate (before relocation) and the primed set for the relocated coordinate. As shown in Fig. 2, a position $x = (x, y)$, which resides outside the domain, belongs to one of the four regions around the domain. For the given $(y, H, t)$, the relocated position $x' = (x', y')$ is determined by the region which $x$ belongs to:

upper zone : $(x', y') = ((x - \gamma H)^+, y - H),$

lower zone : $(x', y') = ((x + \gamma H)^+, y + H),$

right or left zone : $(x', y') = ((1)^+, y),$ otherwise : $(x', y') = (x, y).$

The position $x$ can be either a particle center $X$ or a point on the particle boundary. The last line in Eq. (25) is
introduced to attain the consistency in notation. Since the upper (lower) frame translates faster (slower) than the frame of computation by the amount of $\gamma H$, the relocation involves changes in the $x$ directional velocity component $U$, if a particle crosses upper or lower boundaries. Again the change in the translational velocity can be expressed in a single equation for both a particle center and a point on the particle boundary and is determined by the region where the original (unprimed) position is located:

$$\begin{align*}
\text{upper zone : } U' & = U - \gamma H, \\
\text{lower zone : } U' & = U + \gamma H, \\
\text{otherwise : } U' & = U.
\end{align*}$$

Again, the last line is added for consistency in notation.

3. Numerical methods

3.1. Combined weak formulation with DEVSS/DG

Following the combined weak formulation of Glowinski et al. [2] in which the hydrodynamic force and torque acting on the particle boundary are canceled exactly, we derived the weak form for the Newtonian system together with the rigid-ring description of the particle and with the sliding bi-periodic domain constraints in our previous work [1]. In this work, we extend our previous formulation to incorporate with the viscoelastic fluid. We employ the DEVSS method, a mixed finite-element formulation developed by Guénette and Fortin [5], which appears to provide one of the most robust formulations currently available. The DG formulation of Fortin and Fortin [6] is used for the discretization of the constitutive equation. The combination of the DEVSS formulation with DG has been verified to produce a remarkably stable solution, in particular, for flows with a geometrical singularity [7].

For the DEVSS formulation, we introduce an extra variable $\epsilon$, the viscous polymer stress.

$$\epsilon = 2\eta_D D.$$  

Then one can rewrite the momentum equations for the fluid domain (Eq. (2)) and for the particle domain (Eq. (14)) with the viscous polymer stress, which gives extra stability in the discretized equations compared with the formulation without $\epsilon$.

As we did in the previous work, we introduce three different Lagrangian multipliers $\lambda^h$, $\lambda^v$ and $\lambda^p$, which are associated with the kinematic constraint equation for the periodicity in the horizontal direction (Eq. (8)), the constraint equation for the sliding periodicity in the vertical direction (Eq. (11)) and the rigid-ring constraint along the $i$th particle (Eqs. (6) and (18)):

$$\begin{align*}
\lambda^h & = (\chi^h, \lambda^h) \in L^2(T_h)^2, \\
\lambda^v & = (\chi^v, \lambda^v) \in L^2(T_v)^2, \\
\lambda^p & = (\chi^p, \lambda^p) \in L^2(\partial D(t))^2.
\end{align*}$$

The choice of $T_h$ rather than $T_v$ (or, $T_v$ rather than $T_h$) is arbitrary, but the sign of the multiplier will change according to the choice. In our previous work, we showed that the multipliers $\lambda^h$ and $\lambda^v$ are the traction force on the domain boundary $T$ and that the multiplier $\lambda^p$ is the traction force acting on the particle boundary $\partial D(t)$.

Introducing the separate functional spaces $U$, $P$, $S$ and $E$ for $u$, $p$, $\tau_p$ and $e$, respectively, over the whole domain, including the interior of the particle, the combined weak formulation for the whole domain can be constructed, along with the DG formulation for the constitutive equation. The final weak form can be stated as follows:

For $t > 0$, find $u \in U$, $p \in P$, $\tau_p \in S$, $e \in E$, $\lambda^h \in L^2(T_h)^2$, $\lambda^v \in L^2(T_v)^2$, $\lambda^p \in L^2(\partial D(t))^2$, $U \in \mathbb{R}^2$ and $\omega_0 \in \mathbb{R}$ ($i = 1, \ldots, N$) such that

$$\begin{align*}
&- \int_{T_h} \rho \nabla \cdot \mathbf{w} \, dA + \int_{T_h} 2\eta_D D(u) \cdot D(\mathbf{w}) \, dA - \int_{\partial D(t)} e : D(\mathbf{w}) \, dA \\
&\quad + (\lambda^h, u(0, y) - u(L, y))\mathbf{e}_1 + (\lambda^v, u(x, H, t))\mathbf{e}_2 \\
&\quad - u((x - \gamma H)^+, 0, t)\mathbf{e}_1 + \sum_{i=1}^{N} \lambda^p \mathbf{e}_i \cdot \mathbf{n} - (V_i + \mathbf{x}_i) \\
&\quad \times (x - X_i))|\partial D(t)) = 0, \\
&\int_{T_h} q \nabla \cdot \mathbf{u} \, dA = 0, \\
&\int_{T_h} \mathbf{e}_i : D(u) \, dA + \frac{1}{2\eta_p} \int_{T_h} \mathbf{e}_i : \mathbf{e} \, dA = 0, \\
&\int_{T_h} S \cdot (\mathbf{e}_i + \tau_p - 2\eta_p D(u)) \, dA \\
&\quad - \lambda \sum_i \int_{T_h} S \cdot (\tau_p - \tau_p^{\text{ext}})(\mathbf{u} \cdot \mathbf{n}) \, dA = 0, \\
&\int_{T_h} (\mu^h \cdot u(0, y) - u(L, y))\mathbf{e}_1 = 0.
\end{align*}$$
\[(\mu^*, u(x, H, t) - u((x - y)H^*, 0, t))_i = (\mu^*, f)_v,\]
\[f = (\gamma H, 0),\]  
\[(\mu^*, u = [U_j + \omega_x \times (x - X_i)])_{|\partial E_j} = 0, \quad \forall i = 1, \ldots, N,\]  
\[\tau_{\partial F_j \cap \partial F} = 0 \quad \text{in } \Omega,\]  
for all \(v \in V, q \in P, S \in S, \ell_i \in \mathbb{R}^3 \subset L^2(\Gamma^*)^2, \mu^* \in L^2(\Gamma^*)^2, \mu^* \in L^2(\partial \Omega^*(\ell_i))^2, V_j \in \mathbb{R}^2 \) and \(\xi_i \in \mathbb{R}^N.\)

In Eq. (31), \(\cdot\) is the unit outward normal vector on the boundary of element \(e, \Gamma^*\) is the part of the boundary of element \(e\) where \(\mathbf{n} < 0\), and \(\Gamma_{\partial F_j}^*\) is the neighboring upwind element. The inner product \((\cdot, \cdot)_i\) is the standard inner product in \(L^2(\Gamma^*)^2\):

\[(\mu, v)_i = \int_{\Gamma^*} \mu : v \, ds.\]

We have several remarks on the weak form in Eqs. (28)–(35).

1. The rigid-body motion on the particle boundary is treated as a constraint equation, the rigid-ring constraint, which is satisfied in a weak sense with the multiplier \(\lambda^*\) (Eqs. (28) and (34)), the LIE is satisfied again weakly through the sliding bi-periodic constraints with the multipliers \(\lambda^*\) and \(\lambda^*\) (Eqs. (28), (32) and (33)).

2. The inflow continuity condition of the polymer stress (Eqs. (10) and (13)) on the domain boundary has been treated with the DG formulation (Eq. (31)), by taking the external stress \(\tau_{\partial F_j}^*\) of the element, attached on the domain boundary \(\Gamma^*\), from the stress at the coupled point of the corresponding periodic boundary.

3. The DG method, which uses discontinuous interpolation of the polymer stress, is particularly suited in this simulation not only because of minimal coupling between elements, avoiding a large number of coupled equations, but also from the inherent discontinuous nature of the fictitious domain method, since the viscoelastic stress is discontinuous across the particle boundary.

4. Since the sliding bi-periodic constraints (Eqs. (8) and (13)) impose only the relative relation in the velocity, one needs to specify the reference velocity at a single point in the domain. To obtain the simple shear flow in the \(x\) direction with the upper sliding boundary velocity of \((1/2)\gamma H\) and that of the lower one of \(-(1/2)\gamma H\), we assign a zero value for the velocity in both directions at the center of \(\Gamma^*\).

5. The pressure level of the fluid domain is determined by specifying one of the normal component of the Lagrangian multipliers on \(\partial^*\) or \(\partial^*\), since the multiplier can be identified as the traction force.

6. In the rigid-ring description, the pressure inside the particle is an undetermined constant. Our numerical method with the fictitious domain method chooses a value for the pressure. However, the value of the pressure inside the rigid ring does not affect other results such as the rheological material functions that are presented in Section 4.

(7) When a particle crosses the domain boundary, a part of the particle needs to be relocated as described in Eq. (25), which is possibly followed by the change in the rigid-body motion as mentioned with Eq. (26). In such a situation, Eqs. (28) and (34) need to be modified as follows:

\[(\mu^*(x^*'), u(x^*') - [U_j + \omega_x \times (x - X_i)])_{|\partial E_j} = (\mu^*(x^*'), f')_{|\partial E_j},\]  

where \(f' = (\gamma H, 0)\), when the original \(x^*\) belongs to the upper zone, and it becomes \((\gamma H, 0)\) for \(x^*\) in the lower zone (Fig. 2). (Refer to Hsung et al. [1] for details.)

3.2. Bulk stress

The bulk stress is the average stress over the domain and it can be expressed, for a volume \(V\), as the sum of the fluid contribution and the particle contribution [16]:

\[\langle \sigma \rangle = \frac{1}{V} \int_V \sigma \, dV = \frac{1}{V} \int_{V_f} \sigma \, dV + \frac{1}{V} \int_{V_p} \sigma \, dV,\]

where \(\langle \cdot \rangle\) denotes the averaged quantity in \(V, V_f\) and \(V_p\) are the volume occupied by the fluid and the particle, respectively. For an Oldroyd-B fluid in the absence of inertia, one gets

\[\langle \sigma \rangle = -p' I + 2\mu (D) + \tau' v + \frac{1}{\gamma} \int_{V_p} e A. \]  

In this equation \(p'\) and \(\tau'\) are the averaged contributions of the pressure and the polymer stress from the fluid domain: i.e. \(\int_{V_f} p \, dV / V\) and \(\int_{V_p} p \, dV / V\), respectively. One could evaluate the bulk stress directly from Eq. (37). To do so, one needs the identification of the particle domain, in the regular mesh problem like this, to evaluate \(p'\) and this procedure inevitably involves an additional approximation.

In this regard, we prefer to use an alternative expression, which involves only boundary integrals of the traction force along the domain boundary and on the boundary of particles crossing the domain boundary, as we did in our previous work for the Newtonian system [1]. Since the Lagrangian multipliers \(\lambda^,\lambda^*\), \(\lambda^*\), which are obtained as a part of the solution, can be related directly to the traction forces, the boundary integrals can easily be evaluated. By using the tensor identity \(\lambda \delta_{ij}/\delta \omega = \sigma_{ij}\) in the momentum balance and applying the divergence theorem over the volume \(V\), the bulk stress can be expressed in terms of the traction force on the domain boundary [1]:

\[\langle \sigma \rangle = \frac{1}{V} \int_{V_f} \tau dS + \frac{1}{\gamma} \int_{V_p} e A. \]

The expression in the parenthesis is the 2-D form for the sliding bi-periodic frame of area \(A\).
The identity between the traction force and the Lagrangian multipliers was discussed for the Newtonian system in detail [1]. Such a relationship is still valid in the viscoelastic flow, since the traction force includes the contribution from the polymer stress, $t = n \left( -pI + 2nD + \tau_p \right)$. In this regard, we present the final expression of the bulk stress without proof in the present paper. (Details of the derivation can be found in [1].)

When all particles are completely immersed in the domain (i.e., no boundary-crossing particle), each component of the bulk stress can be obtained by the following equations:

\[
\langle \sigma_1 \rangle = \frac{1}{A} \int_{\partial D} \left( \langle \tau \rangle - x \lambda^s \right) \lambda^q \, dx
+ \frac{1}{L} \int_0^L \lambda^s \lambda^q \, dy,
\]

\[
\langle \sigma_2 \rangle = -\frac{1}{L} \int_0^L \lambda^s \lambda^q \, dx,
\]

\[
\langle \sigma_3 \rangle = \frac{1}{A} \int_{\partial D} \left( \langle \tau \rangle - x \lambda^s \right) \lambda^q \, dx
+ \frac{1}{L} \int_0^L \lambda^s \lambda^q \, dy = -\frac{1}{L} \int_0^L \lambda^s \lambda^q \, dx.
\]

If there are $N_k$ particles crossing the domain boundary, we need a correction term by replacing the particle contribution of the relocated coordinate $x'$ by that of the original coordinate $x$. The bulk stress in this case can be written as follows:

\[
\langle \sigma' \rangle = \langle \sigma \rangle + \frac{1}{A} \sum_{k=1}^{N_k} \left( x - x' \right) \lambda^p \lambda^q \, dx,
\]

where $\langle \sigma' \rangle$ is the result of the boundary integral from Eq. (39). It is worthwhile to notice that the Lagrangian multiplier for the rigidity constraint over the particle domain was identified as a body force in the original DLM method of Glowinski et al. [2] and in its modified version by Patankar et al. [14].

3.3. Implementation

3.3.1. Spatial discretization

For the discretization of the weak form, we use regular quadrilateral elements with continuous bi-quadratic interpolation ($Q_2$) for the velocity $u$, discontinuous linear interpolation ($P_1$) for the pressure $p$, continuous bi-linear interpolation ($Q_1$) for the viscous polymer stress $e$ and discontinuous bi-linear interpolation ($Q_0$) for the polymer stress $\tau_p$. This combination of the discretizations for $u$, $e$ and $\tau_p$ has been verified to give the most stable result with the DEVSS/DG formulation [7]. The use of the discontinuous interpolation of the pressure appears to be mandatory, since an arbitrary location of a particle boundary induces discontinuity in the pressure across the boundary [17].

As we did in Ref. [1], we use point collocation to discretize the weak form of the rigid-ring constraint (Eqs. (28) and (34) or (36)). For example, the integral in Eq. (36) has been approximated as follows:

\[
\left( \mu^p \left( x' \right), u \left( x' \right) \right) - \left( U + \omega_x \left( x - X \right) \right) \lambda_p
\approx \sum_{k=1}^{M} \mu^p \left( \left( x' \right)_k \right) - \left( U + \omega_x \left( x_k - X \right) \right),
\]

where $M$, $x_k$, $x'$ and $\mu^p$ are the number of the collocation points on $\partial P_i$, the original (before relocation) of the $k$th collocation point, the relocated coordinate of the $k$th collocation point and the collocated Lagrangian multiplier at $x'_k$, respectively. We define equally distributed collocation points on the particle boundary based on the original coordinate and the number of the collocation points $M$ is taken to be proportional to the radius of the particle. In our previous work, we analyzed effects of the number of collocation points and found that approximately one collocation point in an element appears to give the most accurate solution [1]. A small change in $M$ from the optimal number does not affect solutions much, but it gives additional control to avoid particle collision, although it hardly occurs in our simulation with a reasonable time step size. (For details, refer to Hwang et al. [1]). In addition, as demonstrated in Eq. (41), the use of point collocation circumvents tedious boundary integrals over the separated particle boundary, when the particle crosses the computational domain.

To discretize the boundary integrals for the horizontal periodicity in Eqs. (28) and (32), we use the nodal collocation method, point collocation at all nodes, since the facing elements between $I_1$ and $I_2$ are always conforming in our simulation with the regular discretization of the computational domain. On the other hand, for the boundary integrals associated with the vertical sliding periodicity (Eqs. (28) and (33)), care should be exercised in choosing a proper discretization of the multiplier $\lambda^v$. The reason is that connection of the facing elements between $I_1$ and $I_2$ are in general non-conforming and time-dependent. The situation is analogous to the mortar/finite element contact description in frictional contact surface problems in solid mechanics, where the traction and kinematic compatibility should be approximated across non-conforming interfaces [18]. In those problems, it has been known that the optimal convergence rate is only obtained when integral representation of the contact constraint based on mortar element methods are utilized [19]. We tested several different interpolations for the multiplier space of $\lambda^v$ in our previous work and we verified that the integral method with continuous linear interpolation of the multiplier space gives the best solutions [1]. We use the same technique in this work.

3.3.2. Time integration

Initially ($t = 0$), the viscoelastic polymer stress is set to be zero over the entire computational domain (Eq. (35)). We
solve the momentum equation with the constraint equations (Eqs. (28)-(30), (32)-(34)) implicitly to get the rigid-body velocity of the particle and the velocity distribution at the initial time step. (See Step 3 with Eq. (44)) below.) Then, at every time step, the following procedures are conducted.

Step 1. Get the particle configuration \( X_{i}^{n+1} \) (i = 1, \ldots, N) by integrating the kinematic equation in Eq. (21) (and Eq. (22)) using the explicit second-order Adams–Bashforth method (AB2):

\[
X_{i}^{n+1} = X_{i}^{n} + \Delta t (\frac{2}{3} U_{i}^{n} - \frac{1}{2} U_{i}^{n-1}).
\]  

(42)

Step 2. Solve the viscoelastic polymer stress \( \tau_{p}^{n+1} \) by integrating the evolution equation of the polymer stress \( \tau_{p} \) (Eq. (31)) using the explicit second-order Adams–Bashforth method (DG/AB2):

\[
[M] \frac{\tau_{p}^{n+1} - \tau_{p}^{n}}{\Delta t} = \frac{3}{4} \mathbf{g} (u^{n}, \tau_{p}^{n}) - \frac{1}{4} \mathbf{g} (u^{n-1}, \tau_{p}^{n-1}).
\]  

(43)

where \([M]\) is the mass matrix and the vector \( \mathbf{g} \) is the forcing term which appears in the evolution equation of \( \tau_{p} \) (Eq. (31)).

Step 3. Get the remaining solutions (\( \eta, p, \epsilon, U, \Omega, \eta_{f}, \lambda_{f}, \lambda^{h} \)) for the \((n+1)\)th step by solving Eqs. (28)-(30) and (32)-(34) implicitly using \( X_{i}^{n+1} \) and \( \tau_{p}^{n+1} \) (i = 1, \ldots, N):

\[
\int_{J_{2}} \rho u^{n+1} \cdot \mathbf{v} \cdot dA + \int_{J_{2}} 2 \eta_{f} D(u^{n+1}) : D(u) \cdot dA
\]

\[
\int_{J_{2}} \epsilon : D(\tau_{p}^{n+1}) \cdot dA + \frac{1}{2} \sum_{n} \int_{J_{2}} \epsilon : \mathbf{d}^{n+1} \cdot dA = 0,
\]  

\[
\left( \mathbf{u}^{n+1}, u^{n+1}_{(0, y)} - u^{n+1}_{(L, y)} \right)_{\Gamma_{1}} = 0,
\]  

\[
\left( \mathbf{u}^{n+1}, u^{n+1}(x, H) - u^{n+1}(x - \gamma H)^{n+1}, 0 \right)_{\Gamma_{1}} = (\mathbf{g}^{n}, f)_{\Gamma_{1}},
\]  

\[
\left( \mathbf{u}^{n+1}, u^{n+1} - \left( U^{n+1} + \omega_{2}^{n+1} \times (x - X^{n+1} ) \right) \right)_{\Gamma_{2}} = 0.
\]  

(44a)

(44b)

(44c)

(44d)

(44e)

(44f)

We have some remarks for each step:

* In the first step, the method needs the present particle position, the previous particle velocity and the present particle velocity to predict the next particle position. However, when the present particle center has come from outside of the upper or lower boundaries via relocation (Eq. (25)), one has to modify the previous velocity according to changes in the x directional translational velocity of the particle (Eq. (26)), since the next particle position should be evaluated based on the present relocated particle position and the present particle velocity. The modification of the AB2 method applies only on the x direction and it can be written, for the ith particle, whose center comes across the upper or lower boundary, as follows:

\[
X_{i}^{n+1} = X_{i}^{n} + \Delta t \left( \frac{2}{3} U_{i}^{n} - \frac{1}{2} U_{i}^{n-1} \right).
\]  

(45)

where \( X_{i}^{n}, X_{i}^{n+1}, U_{i}^{n} \) and \( U_{i}^{n+1} \) are the present (relocated if necessary) particle position, the next particle position, the present velocity, and the modified previous velocity, respectively. The modified previous velocity \( U_{i}^{n-1} \) is determined by Eq. (26) in Section 2.3.

* In the Step 2, Eq. (43) can be solved at the element level, leading to a minimal coupling between elements. In addition, the method provides easy treatments for the external inflow stress \( \tau_{p}^{n+1} \) across the upper and lower sliding boundaries in Eq. (31), which involves the time-dependent non-conforming connection between facing elements. The stability and the second-order accuracy in the solution of the evolution equation of \( \tau_{p} \) with the combination of the DG method in space and the AB2 method in time (DG/AB2) have been verified by Hulsen et al. [20].

* In the last step, Eq. (44) leads to the equation with a sparse symmetric matrix with many zeros on the diagonal, which has been solved by a direct method based on a sparse multifrontal variant of Gaussian elimination (HSLMA41) [21–23].

4. Results

In this section, we present numerical results from the three sets of example problems: a single particle, two particles and six particles in the sliding bi-periodic frame. Because of the bi-periodicity of the computational domain, a few particle system in a single domain represents a large number of particles in an unbounded domain of the same configuration in simple shear flow. There are only two parameters in the Oldroyd-B fluid: the Weissenberg number We and the ratio of the solvent viscosity to the polymer viscosity \( \eta_{f} / \eta_{p} \). The Weissenberg number is defined as

\[
We = \gamma \lambda,
\]

and we use \( \eta_{f} = \eta_{p} \) in all example problems.

Hereafter, for the purpose of the consistency, we will discuss the bulk suspension behavior by presenting the bulk shear stress \( \langle n_{12} \rangle \) and the bulk first normal stress \( \langle N_{11} \rangle \), normalized by \( \eta_{0} \gamma \) and \( 2 \eta_{0} \lambda /\gamma ^{2} \), respectively. In fact, the normalized quantities can be identified by the relative shear vis-
cosity $\eta$ and by the relative first normal stress difference coefficient $\Psi_1$, which can be defined as follows:

$$\eta_r = \frac{\langle \sigma_{12} \rangle}{\eta_0 \dot{\gamma}}, \quad \Psi_1 = \frac{\langle N_1 \rangle}{2\eta_0 \dot{\gamma}^2} = \frac{\langle N_1 \rangle}{2\eta_p \lambda}.$$

(46)

4.1. Single particle in a sliding bi-periodic frame

The first test problem is a single particle of radius $r$ suspended freely at the center of the sliding bi-periodic domain of size $1 \times 1$ (i.e. $L = H = 1$). As mentioned earlier, the reference velocity has been specified by zero at the center of the left domain boundary so that the upper boundary translates at the velocity $\left( \frac{1}{2} \right) \dot{\gamma} H$ and the lower one translates at $-\left( \frac{1}{2} \right) \dot{\gamma} H$. As a result, the particle does not translate relatively to the domain but rotates at the fluctuating angular velocity $\omega(t)$. As shown in Fig. 3, the problem represents a regular configuration of a large number of such a system and the initial configuration of the particle is reproduced periodically with the time period $T = L/\dot{\gamma} H$.

4.1.1. Convergence test

We begin by checking the convergence of our code using the single-particle problem with $r = 0.2$ and $We = 0.5$. We used three different meshes: 25-by-25, 50-by-50 and 100-by-100, denoted by $h = 1/25, 1/50$ and 1/100, respectively. The number of the collocation points on the particle boundary are in turns 32, 64, and 128, which have been verified optimal in our previous work for $r = 0.2$ [1]. Fig. 4 shows the evolution of the angular velocity $\omega$ (normalized by $-\dot{\gamma}$), the relative shear viscosity $\eta_r$ and the relative first normal stress difference $\Psi_1$.

The results show good convergence for all the quantities with mesh refinement. In addition, a smaller time step $\Delta t$ than those used in Fig. 4 gives the same results, although not presented here. The $h = 1/50$ mesh appears to be a proper compromise between the accuracy and the computational costs (in memory and CPU time).

4.1.2. Time-dependent bulk suspension behavior

Since there is no relative change in the particle configuration inside a frame, the single-particle problem appears a good example in investigating the sole effects of the fluid elasticity ($We$) and the solid fraction ($\phi$) on the bulk suspension behavior. At the same time, we want to emphasize that the present results from the single-particle problem which uses the artificial regular particle configuration are different from the suspensions with many particles, especially for
We begin with discussions about the time-dependent behavior of the suspension. Plotted in Fig. 5a–c are the angular velocity of the particle, the relative shear viscosity and the relative first normal stress coefficient of the single-particle problem with $r = 0.2$ for various Weissenberg numbers. All data show temporal fluctuations and converge to steady oscillation for large $t$. The fluctuation originates from the time-periodic change in the relative configuration of the sliding frame as shown in Fig. 3. For example, the magnitude of the angular velocity becomes (local) maximum when the distance between particles (of neighboring upper or lower frames) is minimized, like the initial configuration in Fig. 3, whereas it gives a local minimum value for the configuration of the largest inter-particle distance (the intermediate configuration in Fig. 3.) The relative shear viscosity appears the opposite behavior to the normalized angular velocity: i.e., the viscosity reaches the maximum value when the inter-particle distance (of the upper and lower frames) is the largest, and vice versa. The first normal stress difference reaches the maximum (minimum) value in between the minimum and the maximum inter-particle distances, while the distance decreases (increases). For small Weissenberg number cases, the angular velocity and the bulk shear viscosity converge to the result of the same single-particle problem in the Newtonian fluid. (The Newtonian results were taken from our previous study.)
However, for non-small Weissenberg number cases, we found a remarkable decrease in the absolute value of the angular velocity, about 40% reduction in magnitude of the angular velocity with \( \text{We} = 2.5 \). On the other hand, the shear viscosity and the first normal stress coefficient increase with the Weissenberg number. That is, both properties are shear-thickening. (This issue will be discussed in the next section more details with the time-averaged steady properties.)

In Fig. 6a-c we present those three data with a fixed Weissenberg number (\( \text{We} = 1 \)) for various particle radii. Comparison with the pure fluid case has been made for the bulk shear viscosity and the first normal stress coefficient. For small \( r \), both properties converge to the pure Oldroyd-B fluid results without the particle \( (r = 0) \). All data shows periodic fluctuation, as mentioned before, and the fluctuation amplitude increases with the particle radius. Again, one can find decrease in the absolute value of the angular velocity and increase of the bulk shear viscosity and of the first normal stress coefficient with the increasing particle radius. In the Newtonian system, it is well known that the bulk shear viscosity increases with increasing size of the particle size. The same is true for the viscoelastic system and for the first normal stress coefficient. In fact there is a simple scaling between the first normal stress and the bulk shear stress in suspensions of the Oldroyd-B fluid, which will be discussed in the next section.

### 4.1.3. Steady bulk suspension properties

One can obtain the steady bulk suspension properties by taking the time-average of the steady oscillation parts in the time-dependent behavior of the single-particle results, presented in the previous section. Plotted in Fig. 7a and b are the steady bulk shear viscosity and the first normal stress coefficient evaluated in such a way for several combinations of the Weissenberg numbers and the solid area fractions \( \phi \).

As shown in Fig. 7a, the bulk shear viscosity increases with the Weissenberg number as well as the solid area fraction. That is, the shear viscosity of the bulk suspension shows shear-thickening behavior, when formulated with an Oldroyd-B fluid. For a small Weissenberg number (\( \text{We} = 0.05 \)), the shear viscosity converges to that of the Newtonian system. (The Newtonian results has been adopted from Hwang et al.\[1\].) In addition, for small value of \( \phi \), the shear viscosity of the viscoelastic system converges to Einstein’s analytic result for a dilute Newtonian system, i.e. \( \eta_\infty = 1 + 2\phi \) [24].

The steady time-averaged first normal stress coefficient (Fig. 7b) shows the analogous behavior: it increases with the Weissenberg number and with the solid fraction \( \phi \). In fact, the relative first normal stress coefficient appears shear-thickening and converges to the pure Oldroyd-B fluid result of the value ‘1’ for small \( \phi \). In contrast to the viscoelastic results presented here, the time-averaged value of the first normal stress was found zero in the single-particle problem in the Newtonian system in the sliding bi-periodic frame [1].

Patankar and Hu [26] state that for a 2-D dilute suspension in a second-order fluid (SOF), the relative increase of the viscosity and the first normal stress coefficient due to the presence of the particles is the same and identical to the relative increase of the effective viscosity in the Newtonian
Fig. 8. The ratio of the relative first normal stress difference coefficient to the relative shear viscosity as a function of the solid area fraction for different Weissenberg numbers.

That is, \( \eta_r = 1 + 2\phi \) and \( \Psi_{1r} = 1 + 2\phi \). In order to check the SOF limit, we plotted the ratio of the two, \( \Psi_{1r}/\eta_r \), in Fig. 8. (See also the SOF limit compared in Fig. 7a and b.) Near \( \phi = 0 \), the deviation from 1 seems to be of second order in \( \phi \). For the dilute Oldroyd-B fluid, the SOF limit seems to be fulfilled also up to a moderate Weissenberg number. However, for the non-dilute case, \( \Psi_{1r}/\eta_r > 1 \), i.e. the normal stress increases faster than the shear stress with the solid fraction, (but not as fast as the square of the shear stress, \( \Psi_{1r}/\eta_r^2 < 1 \), which is discussed below.)

Regarding bulk suspension behavior, one common experimental observation is that the first normal stress difference in a filled viscoelastic fluid is a power-law function of the imposed shear stress such that \( N_1 \approx \tau^n \) with an exponent \( n \) that appears to depend on the specific matrix fluid used in preparing the suspensions [8–10]. With this argument, the \( n \) value in the Oldroyd-B fluid becomes 2, since it is independent of the volume fraction. In order to check the appearance of such a relationship in our simulation results, we plotted the steady time-averaged first normal stress difference as a function of the steady bulk shear stress using the log-log scale in Fig. 9. Interestingly, our single-particle simulations in a 2-D sliding frame reveal a set of parallel straight lines which gradually shift to the shear stress axis with increasing solid area fractions, for the wide range of \( \phi \), from the low particle concentration (3.14%) to the extremely high concentration (50.3%). The implication in this plot is that the first normal stress difference relatively decreases with increasing solid area fraction when compared at a constant values of the shear stress. In fact, the first normal stress difference increases with the solid area fraction as shown in Fig. 7b, even faster than the shear stress (see Fig. 8), but not as fast as the square of the shear stress does.

The data in Fig. 9 suggest that the normal stress difference can be conveniently expressed by using a shift factor \( \beta(\phi) \), which only depends on the solid fraction \( \phi \), analogous to the approach of Mall-Gleissle et al. [10]:

\[
\langle N_1 \rangle(\phi, \langle \sigma_{12} \rangle) = \frac{2\eta_p}{\eta_0} \beta(\phi) (\sigma_{12})^2. \tag{47}
\]

With the definition of Eq. (47), \( \beta(\phi = 0) = 1 \). Substituting the definition of \( \eta_r \) and \( \Psi_{1r} \) (Eq. (46)) into Eq. (47), we get

\[
\beta(\phi) = \frac{\Psi_{1r}}{\eta_r}. \tag{48}
\]
In order to show that the right-hand-side of Eq. (48) is indeed independent from the Weissenberg number \( \text{We} \), we have plotted in Fig. 10 the values of \( \Psi_1 / \eta_r \), using the steady time-averaged values of \( \Psi_1 \) and \( \eta_r \), as a function of \( \phi \). The values decrease monotonically within the range of \( \phi \) in our simulations. The dependence on the Weissenberg number is very minor and the approximation by a single function \( \beta(\phi) \) is very good for the values of \( \text{We} \) considered here. In Fig. 10 we have also plotted the SOF limit \( \beta(\phi) = 1/(1 + 2\phi) \), and this simple relation gives a surprisingly good fit for the shift factor up to \( \phi = 0.5 \).

It would be worthwhile to mention the previous results from 2-D direct numerical simulations on bulk suspension properties by Patankar and Hu [25] for a Newtonian fluid and [26] for a viscoelastic fluid. They solved the single-particle problem in a one-side periodic channel under simple shear flow with non-zero Reynolds number (less than 0.035) using a relatively small fluid elasticity (\( \text{We} \) less than 0.2), for a very dilute system (\( \phi \) less than 0.001). They claimed that there is no effect of the fluid elasticity on the bulk viscosity and the first normal stress, as expected from our results in Fig. 7a and b within such a low particle fraction. However, the effect of fluid elasticity on these properties have appeared significant in our present results, as the particle fraction increases and as the fluid elasticity increases.

Before closing the section, it would be interesting to see the steady time-averaged angular velocity of the particle. As indicated in Fig. 11, it decreases substantially with the Weissenberg number and with the solid fraction, and the effect of the Weissenberg number is more pronounced than the solid fraction.

4.2. Two particles in a sliding bi-periodic frame

The two-particle problem is constructed to investigate the effect of the hydrodynamic interaction between two (almost) isolated particles. It is stated as follows: Two identical particles of radius \( r = 0.12 \) are suspended freely in the sliding bi-periodic domain of size 1 \( \times \) 1. The initial positions of the particles are chosen symmetrically as shown in Fig. 12. The distance from the particle center to the horizontal centerline of the domain is denoted by \( D \). Again the reference velocity has been specified by zero at the center of the left domain boundary (\( \Gamma_4 \)) so that the upper left particle is supposed to move to the right direction and the lower right one to the left direction. In fact, the identical problem has been solved in our previous work for suspensions in a Newtonian fluid, where we showed that the bulk viscosity is a function of \( D \) and increases with the averaged inter-particle distance: i.e., minimum for \( D = 0 \) and maximum for \( D = 0.25 \). (Refer to Hwang et al. [1] for details.)

However, in the viscoelastic fluid, we could not perform such a systematic approach to investigate the effect of hydrodynamic interaction, because there is no steady configu-
Fig. 13. The comparison of the orbits of the left particle in the two-particle problem in Newtonian and Oldroyd-B fluids ($D = 0.025$ and $r = 0.12$).

The configuration of the two particle continuously changes. In fact, the motion of the two particles show strong tendency toward clustering. Plotted in Fig. 13 are the orbits of the upper left particle in two Oldroyd-B fluids, $\text{We} = 0.5$ and 1, in comparison with the orbit in a Newtonian fluid for $D = 0.025$. The motion of the other particle is completely symmetric with respect to the point (0.5, 0.5), because of the symmetry of the problem. It is well-known that the closely located two particles show kissing-tumbling-separation phenomena in simple shear flow in the Newtonian fluid, as is also indicated in Fig. 13. However, the figure reveals that the two particles in an Oldroyd-B fluid keep rotating around each other, i.e. we find kissing-tumbling-tumbling-phenomena. In other words, the particles show the tendency for clustering, when they are closely located initially, unlikely to the Newtonian case. As shown in Fig. 13, this tendency appears to get more apparent with the larger Weissenberg number.

Fig. 14. The evolution of the particle configuration in the two-particle problem with $D = 0.025$, $r = 0.12$ and $\text{We} = 0.5$, which shows the kissing-tumbling-tumbling phenomena. The quantity plotted in gray scale is the trace of the polymer conformation tensor $A$ and the particles are described by their collocation points. (a) $\gamma t = 5.75$ ($t/\lambda = 11.5$); (b) $\gamma t = 8.125$; (c) 9.375; (d) 10.25; (e) 14.5; (f) 15.5; (g) 16.875; (h) 19.375; (i) 24.875. The subfigure (g) is near the instant when the two particles are apart the largest (denoted by $\times$ in Fig. 13).

Fig. 15. The comparison of the particle orbits in a Newtonian and an Oldroyd-B ($\text{We} = 0.5$) fluid for $D = 0.05$. The initial position of the particle is marked with a $\times$. 
When the two particles located vertically (as in Fig. 14c), the interaction of the two clustered particles reduces as time goes on. The particles are described by their collocation points. Firstly, the two particles kiss (Fig. 14a and b) and tumble (Fig. 14c and d) and they start to separate (Fig. 14e and f). However, when approaching the maximum separation distance (Fig. 14g), they begin to recoil back (Fig. 14h) and tumble again (Fig. 14i). The whole process repeats continually, reducing the maximum distance between the two particle, as was presented in Fig. 13.

Finally, we present the mesh refinement results for the previous two symmetrically-located-particle problem ($D = 0.025$, $r = 0.12$ and $We = 0.5$), which has been investigated extensively in our paper. In this case, two closely-located particles interact with each other and the accuracy of the solution within the interparticle region is much more involved. We tested three meshes: 25-by-25, 50-by-50 and 100-by-100, denoted by $h = 1/25, 1/50$ and 1/100, respectively, and the comparison has been made for a large number of time steps ($\gamma t \geq 25$), during which the first kissing-tumbling-tumbling phenomena of the two particles occurs. The number of collocation points for each particle (and the time step used) are in turns 24 ($\Delta t = 0.01$), 48 (0.005) and 96 (0.0025) for the $h = 1/25, 1/50$ and 1/100 mesh, respectively. Fig. 18 shows the evolution of the relative viscosity $\eta_r$ and the relative first normal stress difference $\Psi_{rF}$ for the three mesh problems. Plotted in Fig. 19 is the orbit of the left particle for each case. Obviously, the overall behavior does not change significantly with the mesh size. The results indicate good convergence with the mesh refinement, before the instance when the two particles approaches the maximum interparticle distance (near $\gamma t = 15$). (See Fig. 14 for comparison.) Then there appears a small discrepancy in the relative viscosity and the first normal stress difference. The reason is that the particles computed with the finer mesh follow a slightly larger orbit and thereby the time for the particle recoil increases with the mesh refinement. Such a small error is then accumulated for a large number of time steps and causes the phase shift in the bulk stress result later.

4.3. Many particles in a sliding bi-periodic frame

Now we proceed to more complex problems: six randomly distributed particles in the sliding bi-periodic frame. The main objective here is to see how complicated particle–fluid and particle–particle interactions affect the microstructural behavior in concentrated suspensions with a viscoelastic fluid. We consider two different initial configurations of six particles: particles with different radii and with equal radii. The solid area fractions of the two cases are the same ($\phi = 0.296$). Again the size of the sliding frame is $1 \times 1$


\[ 29 \]

\[ \text{The movie files for } We = 0.5 \text{ and } 1 \text{ of the two-particle problem are accompanied with the paper under the names Movie 1 and Movie 2, respectively.} \]

\[ \text{The corresponding movie file is named Movie 3.} \]

![Fig. 16. The location (X,Y) and the rigid-body velocity (U,V,ω) of the left particle in the two-particle problem with $D = 0.025$, $r = 0.12$ and $We = 0.5$. The translational and angular velocity components were normalized by $\gamma h$ and $\gamma$, respectively.} \]
and the reference velocity is specified by zero at the center of the left domain boundary (Γ4). The two initial configurations are plotted in Fig. 20, where the particles are described by their collocation points. The 50-by-50 mesh is used for

Fig. 17. The relative shear viscosity (a) and the relative first normal stress difference coefficient (b) of the two-particle problems in Newtonian and Oldroyd-B fluids (D = 0.025 and r = 0.12).

Fig. 18. The mesh refinement result of the two-interacting-particle problem (D = 0.025, r = 0.12 and We = 0.5). (a) The relative shear viscosity; (b) the relative first normal stress difference coefficient.

Fig. 19. The mesh refinement result of the two-interacting-particle problem (D = 0.025, r = 0.12 and We = 0.5). The orbit of the left particle.

Fig. 20. Two initial particle configurations of different size particles (left) and of the same size particles (right). The two examples have the same solid area fraction φ = 0.296. Particles are described by their collocation points.

the computation and two Weissenberg number flows with We = 0.5 and 1 are tested.

Fig. 21 shows the instantaneous distributions of the trace of tensor A of the different-sized particle case and of the equal-size case for We = 0.5.3 Firstly, one can observe strong elongational flows generated between separating par-

3 A movie file has been prepared for the different sized particle case with We = 0.5 and named Movie 4.
Fig. 21. The distribution of the trace of the conformation tensor in the six-particle problem with $We = 0.5$. (a) The different-sized particle case at $\dot{\gamma}t = 6 \ (\lambda = 12)$ and (b) the equal-sized particle case at $\dot{\gamma}t = 6.3$.

Secondly, another high stretched region occurs when two particles approach (or kiss) each other closely. Thirdly, there is also weak elongational flow region between particles aligned parallel to the flow direction. The value of $\text{tr}(\mathbf{A})$ in such a region is sometimes lower than the value 2.5, which is the value of the pure Oldroyd-B fluid under the same condition. Therefore, the resultant microstructure becomes highly non-uniform and anisotropic. Especially, there seems to be a typical orientation for the highly stretched regions which originate from separating particles. The angle is about 20 [deg.] measured from the flow direction. In addition, such a non-uniform and anisotropic microstructure becomes more pronounced in the higher Weissenberg number flow, as shown in Fig. 22.\(^4\)

The presence of the oriented highly elongational flows is particularly interesting, since it induces polymer molecules to align in such a direction, which could affect the micro-rheological behavior of the suspension. For example, the stretched molecules enhance the nucleation and crystallization process in case of semi-crystalline polymers during processing [27,28], which of course affects the mechanical properties of the final product. (Refer to Schrauwen et al. [11] for experimental observations about flow effects on the impact toughness in the injection-molded products of a hard particle-filled semi-crystalline polymer.)

Finally the relative shear viscosity and the relative first normal stress difference coefficient in the six-particle problems were presented in Fig. 23 along with the comparison with the Newtonian system and with the corresponding single-particle problem having the same solid fraction. (The Newtonian results have been adopted from our previous work [11].) The bulk shear viscosity of the six-particle problem is always larger than that of the corresponding single particle case for both Newtonian and viscoelastic systems, which is the effect of increased hydrodynamic interactions. In addition, there seems to be an increase in the relative viscosity with the Weissenberg number, which agrees with the single-particle result in Fig. 7a. However, due to too much fluctuations in our data, we postpone the conclusion on the other parameter dependencies: e.g., dependence of the first normal stress coefficient on the strength of hydrodynamic interaction and on the Weissenberg number. Computations with a large number of particles for a long time seem to be necessary to investigate definite relations on such matters.

\(^4\)The corresponding movie file has been prepared and named Movie S.
5. Conclusions

In this work, a new finite-element formulation for direct numerical simulations of particle suspensions in an Oldroyd-B fluid has been developed and implemented, by extending the authors’ previous scheme for suspensions in the Newtonian fluid. The main features of our present scheme can be summarized as follows:

- The sliding bi-periodic domain concept of Lees and Edwards for discrete particles has been extended to continuous field problems and combined with the DEVSS/DG finite-element method for accurate and stable computation of viscoelastic flows.
- The freely suspended particles are described by the rigid-ring problem, which eliminates the need for particle domain discretization and allows easy treatment of the boundary-crossing particles.
- A simple expression of the bulk stress has been established, which involves only boundary integrals of the Lagrangian multipliers along the domain boundary and along the boundary of particles crossing the domain boundary.

Concentrating on 2-D circular disk particles, we discussed the bulk rheology of the suspensions and the micro-structural developments through the numerical examples of single-, two- and many-particle problems, which represents a large number of such systems in the unbounded domain. Below are the summary of our observations from the example problems:

- From the single-particle problems, we reported the bulk shear viscosity and the first normal stress difference coefficient, from very dilute to highly concentrated suspensions. Both of them show shear-thickening behavior. The common experimental scaling of the first normal stress to the bulk shear stress has been reproduced.
- Clustering of the two particles has been reported, which is quite distinct from the Newtonian system, and the tendency of such phenomena has been found to increase with the elasticity in the fluid.
- From the many-particle problems, we observed the presence of strong elongational flows between separating particles, which leads to highly oriented and non-uniform micro-structures in suspensions of the viscoelastic flows.

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