A 3D DLM/FD method for simulating the motion of spheres in a bounded shear flow of Oldroyd-B fluids

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Abstract

We present a novel distributed Lagrange multiplier/fictitious domain (DLM/FD) method for simulating fluid-particle interaction in Oldroyd-B fluids under creeping conditions. The results concerning two ball interaction in a three dimensional (3D) bounded shear flow are obtained for Weissenberg numbers up to 1. The pass and return trajectories of the two ball mass centers are similar to those in a Newtonian fluid; but they lose the symmetry due to the effect of elastic force arising from viscoelastic fluids. A tumbling chain of two balls (a dipole) may occur, depending on the value of the Weissenberg number and the initial vertical displacement of the ball mass center to the middle plane between two walls.

Keywords: Oldroyd-B fluid; Shear flow; Neutrally buoyant particles; Distributed Lagrange multiplier/fictitious domain methods.

1 Introduction

Particles suspended in flowing fluids occur in many engineering and biological systems. The rheological behavior of suspensions has been studied heavily during recent decades (e.g., see \cite{1} for the overview of the rheology of suspensions). For the dynamics of rigid non-Brownian particles suspended in viscoelastic fluids, D’Avino and Maffettone have reviewed the existing literature in \cite{2} with focus on theoretical predictions, experimental observations and numerical simulations of peculiar phenomena induced by fluid elasticity which dramatically affects the particle motion and patterning. In Newtonian fluids, random displacements resulting from particle encounters under creeping conditions lead to hydrodynamically induced particle migration, which constitutes an important mechanism for particle redistribution in the suspending fluid (see, e.g., \cite{3} and the references therein). But particle suspensions in viscoelastic fluids have different behaviors, e.g., strings of spherical particles aligned in the flow direction (e.g., see \cite{4,5,6,7}) and 2D crystalline patches of particles along the flow direction.
direction \[8\] in shear flow. As mentioned in \[9\], these flow-induced self-assembly phenomena have great potency for creating ordered macroscopic structures by exploiting the complex rheological properties of the suspending fluid as driving forces, such as its shear-thinning and elasticity. To understand more about particle interaction in viscoelastic fluids, Snijkers et al. \[9\] have studied experimentally the two ball interaction in Couette flow of viscoelastic fluids in order to understand flow-induced assembly behavior associated with the string formation. They obtained that, in high-elasticity Boger fluid, the pass trajectories have a zero radial shift, but are not completely symmetric. In a wormlike micellar surfactant with a single dominant relaxation time and a broad spectrum shear-thinning elastic polymer solution, interactions are highly asymmetric and both pass and return trajectories have been obtained. Based on their observation, shear-thinning of the viscosity seems to be the key rheological parameter that determines the overall nature of the hydrodynamical interactions, rather than the relative magnitude of the normal stress differences. Same conclusion about the role of shear-thinning on the aggregation of many particles has been reported in \[5, 6\]. There are numerical studies of the two particle interaction and aggregation in viscoelastic fluids. For example, Hwang et al. \[10\] applied a finite element method to perform a two-dimensional (2D) computational study and obtained the existence of complex kissing-tumbling-tumbling interactions for two disks in an Oldroyd-B fluid in sliding bi-periodic frames: The two circular disks keep rotating around each other while their centers come closer to each other. Choi et al. \[11\] used an extended finite element method (a methodology introduced in Moës et al. \[12\]) to simulate two circular particles in a 2D bounded shear flow between two moving walls for a Giesekus fluid: Besides the fact that the two disks either pass each other, have reversing trajectories (return) or rotate as a pair (tumble), they also had another interaction, namely, the two disks rotate at a constant speed with their mass centers remaining at a fixed position. To simulate the interaction of two spherical particles interacting in an Oldroyd-B fluid, Yoon et al. \[13\] applied a finite element method to discretize the fluid flow with a discontinuous Galerkin approximation for the polymer stress: In their numerical approach, the rigid property of the particles is imposed by treating them as a fluid having a much higher viscosity than the surrounding fluid. They obtained that, for the two balls initially located in the same vorticity plane, the balls either pass, return, or tumble in a bounded shear flow driven by two moving walls for the Weissenberg number up to 0.3. To study numerically the alignment of two and three balls in a viscoelastic fluid, Jaensson et al. \[14\] developed a computational method which mainly combines the finite element method, the arbitrary Lagrange-Euler method \[15\], the log-conformation representation for the conformation tensor \[16 \[17\], SUPG stabilization \[18\] and second-order time integration schemes. Using such computational method, they simulated the motion of two and three balls in bounded shear flows of a viscoelastic fluid of Giesekus type with the effect of the shear-thinning. They concluded that the presence of normal stress differences is essential for particle alignment to occur, although it is strongly promoted by shear.
To simulate the interaction of neutrally buoyant balls in a bounded shear flow of Oldroyd-B fluids in three dimensions (3D), we have generalized a DLM/FD method developed in [19] for simulating the motion of neutrally buoyant particles in Stokes flows of Newtonian fluids to 3D and then combined such method with an operator splitting scheme and a matrix-factorization approach for treating numerically the constitutive equations of the conformation tensor of Oldroyd-B fluids. In this matrix-factorization approach [20], which is a technique closely related to the one developed by Lozinski and Owens in [21], we solve the equivalent equations for the conformation tensor so that the positive definiteness of the conformation tensor at the discrete time level can be preserved. This aforementioned method has been validated by comparing the numerical results of the ball rotating velocity in shear flow with the available results in literature. For the encounter of two balls in a bounded shear flow, the trajectories of the two ball mass centers are consistent with those obtained in [13].

We have further tested the cases of two ball interaction for the Weissenberg number up to 1; our results show the two balls either passing, returning, or tumbling in a bounded shear flow driven by two moving walls. The passing over/under trajectories of the two ball mass centers loses its symmetry due to the effect of the elastic force arising from Oldroyd-B fluids. While two balls form a chain and then tumble in a shear flow driven by two walls, the tumbling motion can change to kayaking for higher Wi. The content of the article is as follows: We discuss the DLM/FD formulation and then the related numerical schemes in Section 2. In Section 3, we first validate our methodology by comparing numerical results for particle motion with those available in literature. We also present the results of numerical simulations investigating the interaction of two balls in a bounded shear flow. Conclusions are summarized in Section 4.

2 Models and numerical methods

2.1 DLM/FD formulation

Fictitious domain formulations using distributed Lagrange multiplier for flow around freely moving particles at finite Reynolds numbers and their associated computational methods have been developed and tested in, e.g., [22, 23, 24, 25, 26, 27, 28]. For the cases of a neutrally buoyant particle in two-dimensional fluid flows of a Newtonian fluid at the Stokes regime, a similar DLM/FD method has been developed and validated in [19]. In this section, we discuss first the formulation for the case of a ball and then the associated numerical treatments for simulating its motion in a 3D bounded shear flow of Oldroyd-B fluids. Let \( \Omega \subset \mathbb{R}^3 \) be a rectangular parallelepiped filled with an Oldroyd-B fluid and containing a freely moving rigid sphere \( B \) centered at \( G = \{G_1, G_2, G_3\}^t \). The governing equations are presented in the following
\[
\begin{align*}
- \nabla \cdot \sigma^s - \nabla \cdot \tau &= g \quad \text{in} \quad \Omega \setminus \overline{B(t)}, \quad t \in (0, T), \quad (1) \\
\nabla \cdot u &= 0 \quad \text{in} \quad \Omega \setminus \overline{B(t)}, \quad t \in (0, T), \quad (2) \\
u &= g_0 \quad \text{on} \quad \Gamma \times (0, T), \quad \text{with} \quad \int_{\Gamma} g_0 \cdot n \, d\Gamma = 0, \quad (3) \\
\frac{\partial C}{\partial t} + (u \cdot \nabla) C - (\nabla u) C - C (\nabla u)^t &= -\frac{1}{\lambda_1} (C - I) \quad \text{in} \quad \Omega \setminus \overline{B(t)}, \quad (4) \\
C(x, 0) &= C_0(x), \quad x \in \Omega \setminus \overline{B(0)}, \quad C = C_L \quad \text{on} \quad \Gamma^- . \quad (5)
\end{align*}
\]

In (1), \(g\) denotes gravity and the Cauchy stress tensor \(\sigma\) is splitted into two parts, a Newtonian (solvent) part \(\sigma^s\) and a viscoelastic part \(\tau\), with:

\[
\begin{align*}
\sigma^s &= -p I + 2\mu D(u), \\
\tau &= \frac{\eta}{\lambda_1} (C - I),
\end{align*}
\]

where \(D(u) = (\nabla u + (\nabla u)^t)/2\) is the rate of deformation tensor, \(u\) is the flow velocity, \(p\) is the pressure, \(C\) is the conformation tensor, \(I\) is the identity tensor, \(\mu = \eta_1\lambda_2/\lambda_1\) is the solvent viscosity of the fluid, \(\eta = \eta_1 - \mu\) is the elastic viscosity of the fluid, \(\eta_1\) is the fluid viscosity, \(\lambda_1\) is the relaxation time of the fluid, and \(\lambda_2\) is the retardation time of the fluid. The conformation tensor \(C\) is symmetric and positive definite (see, e.g., [29]). In (3), \(\Gamma\) is the union of the bottom boundary \(\Gamma_1\) and top boundary \(\Gamma_2\) as in Figure 1 and \(n\) is the unit normal vector pointing outward to the flow region, \(\Gamma^- (t)\) in (4) being the upstream portion of \(\Gamma\) at time \(t\). The boundary conditions given in (3) are \(g_0 = \{-U, 0, 0\}^t\) on \(\Gamma_1\) and \(g_0 = \{U, 0, 0\}^t\) on \(\Gamma_2\) for a bounded shear flow. We assume also that the flow is periodic in the \(x_1\) and \(x_2\) directions with the periods \(L_1\) and \(L_2\), respectively, a no-slip condition taking place on the boundary of the particle \(\gamma (\d \partial B)\), namely

\[
u(x,t) = V(t) + \omega(t) \times \overline{G(t)x}, \quad \forall \ x \in \partial B(t), \quad t \in (0, T)
\]
with $G(t)\mathbf{x} = \{x_1 - G_1(t), x_2 - G_2(t), x_3 - G_3(t)\}^t$. In addition to (6), the motion of particle $B$ satisfies the following Euler-Newton’s equations

$$\frac{dG}{dt} = \mathbf{V},$$

$$\frac{d\theta}{dt} = \mathbf{\omega},$$

$$M_p \frac{d\mathbf{V}}{dt} = M_p \mathbf{g} + \mathbf{F}_H,$$

$$I_p \frac{d\mathbf{\omega}}{dt} = \mathbf{T}_H,$$

$$\mathbf{V}(0) = \mathbf{V}_0, \quad \mathbf{\omega}(0) = \mathbf{\omega}_0, \quad G(0) = G_0, \quad \theta(0) = \theta_0,$$

where $M_p$ and $I_p$ are the mass and inertia tensor of $B$, respectively, $\mathbf{V}$ is the velocity of the center of mass, $\mathbf{\omega}$ is the angular velocity and $\theta$ is the inclination angle of the particle. The hydrodynamical forces and torque are given by

$$\mathbf{F}_H = - \int_{\partial B} \sigma \mathbf{n} ds, \quad \mathbf{T}_H = - \int_{\partial B} \overrightarrow{Gx} \times \sigma \mathbf{n} ds.$$

To obtain a distributed Lagrange multiplier/fictitious domain formulation for the above problem (1)–(12), we proceed as in [22, 24], namely: (i) we derive first a global variational formulation (of the virtual power type) of problem (1) –(12), (ii) we then fill the region occupied by the rigid body by the surrounding fluid (i.e., embed $\Omega \setminus \overline{B(t)}$ in $\Omega$) with the constraint that the fluid inside the rigid body region has a rigid body motion, and then (iii) we relax the rigid body motion constraint by using a distributed Lagrange multiplier, obtaining thus the following fictitious domain formulation over the entire region $\Omega$:

For a.e. $t \in (0,T)$, find $\mathbf{u}(t) \in \mathbf{V}_{g_0}$, $p(t) \in L_0^2(\Omega)$, $\mathbf{C}(t) \in \mathbf{V}_{C_L(t)}$, $\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\mathbf{\omega}(t) \in \mathbb{R}^3$, $\mathbf{\lambda}(t) \in \Lambda(t)$ such that

$$\begin{cases}
- \int_{\Omega} p \nabla \cdot \mathbf{v} d\mathbf{x} + 2\mu \int_{\Omega} \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v}) d\mathbf{x} - \int_{\Omega} (\nabla \cdot \mathbf{\tau}) \cdot \mathbf{v} d\mathbf{x} \\
- \mathbf{\lambda} \cdot \mathbf{v} - \mathbf{Y} - \mathbf{\xi} \times \overrightarrow{Gx} >_{\Lambda(t)} + M_p \frac{d\mathbf{V}}{dt} \cdot \mathbf{Y} + I_p \frac{d\mathbf{\omega}}{dt} \cdot \mathbf{\xi} \\
= (1 - \frac{\rho_f}{\rho_s})M_p \mathbf{g} \cdot \mathbf{Y} + \rho_f \int_{\Omega} \mathbf{g} \cdot \mathbf{v} d\mathbf{x}, \quad \forall \mathbf{v} \in \mathbf{V}_0, \quad \forall \mathbf{Y} \in \mathbb{R}^3, \quad \forall \mathbf{\xi} \in \mathbb{R}^3,
\end{cases}$$

(13)
\[
\int_{\Omega} q \, \nabla \cdot u(t) \, dx = 0, \quad \forall q \in L^2(\Omega),
\]

(14)

\[
< \mu, u(t) - V(t) - \omega(t) \times G >_{\Lambda(t)} = 0, \quad \forall \mu \in \Lambda(t),
\]

(15)

\[
\int_{\Omega} \left( \frac{\partial C}{\partial t} + (u \cdot \nabla) C - (\nabla u) C - C(\nabla u)^t \right) : s \, dx
\]

\[
= - \int_{\Omega} \frac{1}{\lambda_1} (C - I) : s \, dx, \quad \forall s \in V_{C_0}, \text{with } C = I \text{ in } B(t),
\]

(16)

\[
d_G \frac{dt}{dt} = V,
\]

(17)

\[
C(x, 0) = C_0(x), \quad \forall x \in \Omega, \text{with } C_0 = I \text{ in } B(0),
\]

(18)

\[
G(0) = G_0, \quad V(0) = V_0, \quad \omega(0) = \omega_0, \quad B(0) = B_0,
\]

(19)

where the function spaces in problem (13)–(19) are defined by

\[
V_{g_0} = \{ v | v \in (H^1(\Omega))^3, \ v = g_0 \text{ on } \Gamma, \text{ v is periodic in the } x_1 \text{ and } x_2 \\
\text{ directions with periods } L_1 \text{ and } L_2, \text{ respectively} \},
\]

\[
V_0 = \{ v | v \in (H^1(\Omega))^3, \ v = 0 \text{ on } \Gamma, \text{ v is periodic in the } x_1 \text{ and } x_2 \\
\text{ directions with periods } L_1 \text{ and } L_2, \text{ respectively} \},
\]

\[
L^2_0(\Omega) = \{ q | q \in L^2(\Omega), \int_{\Omega} q \, dx = 0 \},
\]

\[
V_{C_L(t)} = \{ C \ | \ C \in (H^1(\Omega))^{3 \times 3}, \ C = C_L(t) \text{ on } \Gamma^- \},
\]

\[
V_{C_0} = \{ C \ | \ C \in (H^1(\Omega))^{3 \times 3}, \ C = 0 \text{ on } \Gamma^- \},
\]

\[
\Lambda(t) = (H^1(B(t)))^3,
\]

and for any \( \mu \in H^1(B(t))^3 \) and any \( v \in V_0 \), the pairing \( < \cdot, \cdot >_{\Lambda(t)} \) in (13) and (15) is defined by

\[
< \mu, v >_{\Lambda(t)} = \int_{B(t)} (\mu \cdot v + d^2 \nabla \mu : \nabla v) \, dx
\]

where \( d \) is a scaling constant, a typical choice for \( d \) being the diameter of particle \( B \).

Remark 1. In relation (13) we can replace \( 2 \int_{\Omega} D(u) : D(v) \, dx \) by \( \int_{\Omega} \nabla u : \nabla v \, dx \). Also the gravity term \( g \) in (13) can be absorbed into the pressure term.

Remark 2. In the system (13)–(19), the treatment of neutrally buoyant particles is quite different from those considered in, e.g., [26, 27] for the cases of neutrally buoyant particles in incompressible viscous flow modeled by the full Navier-Stokes equations. For the particle-flow interaction under creeping flow conditions considered in this article, there is no need to add any extra constraint on the Lagrange multiplier as in [26, 27].
2.2 Numerical methods

For the space discretization, we have chosen $P_1$-iso-$P_2$ and $P_1$ finite element spaces for the velocity field and pressure, respectively, (like in Bristeau et al. [30] and Glowinski [25]), that is

$$W_h = \{ \mathbf{v}_h | \mathbf{v}_h \in (C^0(\Omega))^3, \mathbf{v}_h|_T \in (P_1)^3, \forall T \in \mathcal{T}_h, \mathbf{v}_h \text{ is periodic in the } x_1 \text{ and } x_2 \text{ directions with the periods } L_1 \text{ and } L_2, \text{ respectively} \},$$

$$W_{0h} = \{ \mathbf{v}_h | v_h \in W_h, \mathbf{v}_h = \mathbf{0} \text{ on } \Gamma \},$$

$$L^2_h = \{ q_h | q_h \in C^0(\bar{\Omega}), q_h|_T \in P_1, \forall T \in \mathcal{T}_2h, q_h \text{ is periodic in the } x_1 \text{ and } x_2 \text{ directions with the periods } L_1 \text{ and } L_2, \text{ respectively} \},$$

$$L^2_{0h} = \{ q_h | q_h \in L^2_h, \int_\Omega q_h \, dx = 0 \},$$

where $h$ is the space discretization mesh size, $\mathcal{T}_h$ is a regular tetrahedral mesh covering $\Omega$, $\mathcal{T}_2h$ is another tetrahedral mesh also covering $\Omega$, twice coarser than $\mathcal{T}_h$, and $P_1$ is the space of the polynomials in three variables of degree $\leq 1$.

The finite dimensional spaces for approximating $V_{C_{L(t)}}$ and $V_{C_0}$, respectively, are defined by

$$V_{C_{L(t)}} = \{ \mathbf{s}_h | \mathbf{s}_h \in (C^0(\bar{\Omega}))^{3\times 3}, \mathbf{s}_h|_T \in (P_1)^{3\times 3}, \forall T \in \mathcal{T}_h, \mathbf{s}_h|_{\Gamma^-} = C_{L_h}(t), \mathbf{s}_h \text{ is periodic in the } x_1 \text{ and } x_2 \text{ directions with the periods } L_1 \text{ and } L_2, \text{ respectively} \},$$

$$V_{C_{0h}} = \{ \mathbf{s}_h | \mathbf{s}_h \in (C^0(\bar{\Omega}))^{3\times 3}, \mathbf{s}_h|_T \in (P_1)^{3\times 3}, \forall T \in \mathcal{T}_h, \mathbf{s}_h|_{\Gamma^-} = \mathbf{0} \mathbf{s}_h \text{ is periodic in the } x_1 \text{ and } x_2 \text{ directions with the periods } L_1 \text{ and } L_2, \text{ respectively} \},$$

where $\Gamma^- = \{ x | x \in \Gamma, \mathbf{g}_{0h}(x) \cdot \mathbf{n}(x) < 0 \}$.

For simulating the particle motion in fluid flows, a typical finite dimensional space approximating $\Lambda(t)$ (e.g., see [24, 27, 28]) is defined as follows: let $\{y_i \}_{i=1}^{N(t)}$ be
The above approximate delta functions measure \( \delta \) the velocity field, \( \{X\} \) with \( \partial B \) of \( \mu \) function < we have modified the discrete pairing by

\[
\Lambda_h(t) = \{ \mu_h | \mu_h = \sum_{i=1}^{N(t)} \mu_i \delta(x - y_i), \ \mu_i \in \mathbb{R}^3, \ \forall i = 1, ..., N(t) \},
\]

where \( \delta(\cdot) \) is the Dirac measure at \( x = 0 \). Then, we define a pairing over \( \Lambda_h(t) \times W_{0h} \) by

\[
< \mu_h, v_h >_{\Lambda_h(t)} = \sum_{i=1}^{N(t)} \mu_i \cdot v_h(y_i), \ \forall \mu_h \in \Lambda_h(t), \ v_h \in W_{0h}.
\]

A typical set \( \{y_j\}_{j=1}^{N(t)} \) of the points of \( \overline{B}(t) \) to be used in (21) is defined as

\[
\{y_j\}_{j=1}^{N(t)} = \{y_j\}_{j=1}^{N(t)} \cup \{y_j\}_{j=N(t)+1}^{N(t)+N_1(t) + 1}
\]

where \( \{y_j\}_{j=1}^{N(t)} \) (resp., \( \{y_j\}_{j=N(t)+1}^{N(t)+N_1(t) + 1} \) is the set of those vertices of the velocity grid \( T_h \) contained in \( B(t) \) and whose distance to \( \partial B(t) \geq h/2 \) (resp., is a set of selected points of \( \partial B(t) \), as shown in Fig. [2]. But for simulating particle interactions in Stokes flow, we have modified the discrete pairing \( < \cdot, \cdot >_{\Lambda_h(t)} \) as follows:

\[
< \mu_h, v_h >_{\Lambda_h(t)} = \sum_{i=1}^{N(t)} \mu_i \cdot v_h(y_i) + \sum_{i=N(t)+1}^{M} \sum_{j=1}^{N(t)} \mu_i \cdot v_h(y_i) D_h(y_i - x_j) h^3,
\]

for \( \mu_h \in \Lambda_h(t) \) and \( v_h \in W_{0h} \) where \( h \) is the uniform finite element mesh size for the velocity field, \( \{x_j\}_{j=1}^{M} \) is the set of the grid points of the velocity field, and the function \( D_h(X - \xi) \) is defined as

\[
D_h(X - \xi) = \delta_h(X_1 - \xi_1)\delta_h(X_2 - \xi_2)\delta_h(X_3 - \xi_3)
\]

with \( X = \{X_1, X_2, X_3\}^t \), \( \xi = \{\xi_1, \xi_2, \xi_3\}^t \), the one–dimensional approximate Dirac measure \( \delta_h \) being defined by

\[
\delta_h(s) = \begin{cases} 
\frac{1}{8h} \left( 3 - \frac{2|s|}{h} + \sqrt{1 + \frac{4|s|}{h} - 4\left(\frac{|s|}{h}\right)^2} \right), & |s| \leq h, \\
\frac{1}{8h} \left( 5 - \frac{2|s|}{h} - \sqrt{-7 + \frac{12|s|}{h} - 4\left(\frac{|s|}{h}\right)^2} \right), & h \leq |s| \leq 2h, \\
0, & \text{otherwise}.
\end{cases}
\]

The above approximate delta functions \( \delta_h \) and \( D_h \) are the typical ones used in the popular immersed boundary method developed by Peskin, e.g., [31, 32, 33].

To fully discretize system (13)–(19), we reduce it first to a finite dimensional initial value problem using the above finite element spaces (after dropping most of the sub-scripts \( h \)'s). Next, we combine the Lozinski-Owens factorization approach
Finally we obtain thus the following sequence of sub-problems (where and apply the backward Euler schemes to time-discretize some of these subproblems. The above finite element analogue of system (13)–(19) into a sequence of subproblems (see, e.g., [21], [20]) with the Lie scheme (e.g., see [34], [35], and [36]) to decouple the time-discretization step and time $\Delta t(> 0)$ is a time-discretization step and $t^n = n\Delta t$):

$$C^0 = C_0, G^0 = G_0, V^0 = V_0, \text{and } \omega^0 = \omega_0 \text{ are given;}$$

(25)

For $n \geq 0$, $C^n, G^n, V^n, \omega^n$ being known, we compute the approximate solution at $t = t^{n+1}$ via the following fractional steps:

1. We first predict the position and the translation velocity of the center of mass as follows:

$$\frac{dG}{dt} = V(t),$$

(26)

$$M_p \frac{dV}{dt} = 0,$$

(27)

$$I_p \frac{d\omega}{dt} = 0,$$

(28)

$$V(t^n) = V^n, \omega(t^n) = \omega^n, G(t^n) = G^n,$$

(29)

for $t^n < t < t^{n+1}$. Then set $V^{n+\frac{1}{2}} = V(t^{n+1}), \omega^{n+\frac{1}{2}} = \omega(t^{n+1}),$ and $G^{n+\frac{1}{2}} = G(t^{n+1})$. After the center $G^{n+\frac{1}{2}}$ is known, the position $B^{n+\frac{1}{2}}$ occupied by the particle is determined.

2. Next, we enforce the rigid body motion in $B^{n+\frac{1}{2}}$ and solve for $u^{n+\frac{1}{2}}, p^{n+\frac{1}{2}}, V^{n+\frac{1}{2}}$ and $\omega^{n+\frac{1}{2}}$ simultaneously as follows:

Find $u^{n+\frac{1}{2}} \in W_h, u^{n+\frac{1}{2}} = g_{0h}$ on $\Gamma$, $p^{n+\frac{1}{2}} \in L^2_{0h}, \lambda^{n+\frac{1}{2}} \in \Lambda_{h+\frac{1}{2}}, V^{n+\frac{1}{2}} \in \mathbb{R}^3, \omega^{n+\frac{1}{2}} \in \mathbb{R}^3$ so that

$$\left\{ \begin{array}{l}
- \int_\Omega p^{n+\frac{1}{2}} \nabla \cdot v dx + \mu \int_\Omega \nabla u^{n+\frac{1}{2}} : \nabla v dx - \int_\Omega (\nabla \cdot \frac{\eta}{\lambda_1} (C^n - I)) \cdot v dx \\
+ M_p \frac{V^{n+\frac{1}{2}} - V^{n+\frac{1}{2}} - 2 \omega^{n+\frac{1}{2}} - \omega^{n+\frac{1}{2}}}{\Delta t} \cdot \xi \\
= (1 - \frac{\rho t}{\rho_s}) M_p g \cdot \lambda + \lambda^{n+\frac{1}{2}} \times \xi \times \frac{G^{n+\frac{1}{2}}}{\Lambda_{h+\frac{1}{2}}} > 0,
\end{array} \right.$$ (30)

$$\forall v \in W_{0h}, \lambda \in \mathbb{R}^3, \xi \in \mathbb{R}^3,$$

$$\int_\Omega q \nabla \cdot u^{n+\frac{1}{2}} dx = 0, \forall q \in L^2_h,$$

(31)

$$< \mu, u^{n+\frac{1}{2}} - V^{n+\frac{1}{2}} - \omega^{n+\frac{1}{2}} \times \frac{G^{n+\frac{1}{2}}}{\Lambda_{h+\frac{1}{2}}} > = 0, \forall \mu \in \Lambda_{h+\frac{1}{2}}.$$ (32)
3. We then compute $A^{n+\frac{3}{4}}$ via the solution of

$$\begin{cases}
\int_{\Omega} \frac{\partial A(t)}{\partial t} : s \, dx + \int_{\Omega} (u^{n+\frac{3}{4}} \cdot \nabla) A(t) : s \, dx = 0, \forall s \in V_{Ah}, \\
A(t^n) = A^n, \text{ where } A^n(A^n)^t = C^n, \\
A(t) \in V_{A_{Lh}}^{n+1}, t \in [t^n, t^{n+1}],
\end{cases}$$

and set $A^{n+\frac{3}{4}} = A(t^{n+1})$.

4. Finally we obtain $A^{n+1}$ via the solution of

$$\begin{cases}
\int_{\Omega} \left( \frac{A^{n+1} - A^{n+\frac{3}{4}}}{\Delta t} - (\nabla u^{n+\frac{3}{4}}) A^{n+1} + \frac{1}{2\lambda_1} A^{n+1} \right) : s \, dx = 0, \\
\forall s \in V_{Ah}, A^{n+1} \in V_{A_{Lh}}^{n+1},
\end{cases}$$

and set

$$C^{n+1} = A^{n+1}(A^{n+1})^t + \frac{\Delta t}{\lambda_1} I, \text{ and then } C^{n+1} = I \text{ in } B^{n+\frac{3}{4}}.$$ (35)

Set $G^{n+1} = G^{n+\frac{3}{4}}$, $V^{n+1} = V^{n+\frac{3}{4}}$, and $\omega^{n+1} = \omega^{n+\frac{3}{4}}$.

In (33)-(35), the space $V_{A_{Lh}}^{n+1}$ is $V_{A_{Lh}}(t^{n+1})$, $V_{A_{Lh}}(t)$ and $V_{Ah}$ being defined similarly to $V_{C_{Lh}}(t)$ and $V_{C_{Ah}}$. The multiplier space $\Lambda^{n+\frac{3}{4}}_h$ in (30)-(32) is defined according to the position of $B^{n+\frac{3}{4}}$.

**Remark 3.** When simulating the motion of balls in a Newtonian fluid, we skip problems (33), (34) and (35) in algorithm (26)-(35) and set the elastic viscosity of the fluid to zero.

### 2.3 On the solution of the subproblems

At the steps 3 and 4 of algorithm (26)-(35), we have considered the equations verified by $A$ instead of those verified by the conformation tensor $C$ due to the use of a factorization approach (e.g., see [20] for details). In the implementation, this kind of the Lozinski-Owens’ scheme relies on the matrix factorization $C = AA^T$ of the conformation tensor, and then on a reformulation in terms of $A$ of the time dependent equation modelling the evolution of $C$, providing automatically that $C$ is at least positive semi-definite (and symmetric). The matrix factorization based method introduced in [21] has been applied, via an operator splitting scheme coupled to a FD/DLM method, to the simulation of two-dimensional particulate flows of Oldroyd-B and FENE fluids in [20, 37].
The equation (33) is a pure advection problem. We solve this equation by a wave-like equation method (see, e.g., [25], [38], and [20] (p. 102)) which is a numerical dissipation free explicit method. Since the advection problem is decoupled from the others, we can choose a proper sub-time step so that the CFL condition is satisfied. Problem (33) gives a simple equation at each grid point which can be solved easily if we use trapezoidal quadrature rule to compute the integrals. The value of $\nabla u^n$ at each interior grid node is obtained by the averaged value of those values computed in all tetrahedral elements having the grid node as a vertex, however for the grid node on $\Gamma$ it is obtained by applying linear extrapolation via the values of two neighboring interior nodes as discussed in [39].

Problem (26)-(29) is just a system of ordinary differential equations. They are solved using the forward Euler method with a sub-time step to predict the translation velocity of the mass center and then the position of the mass center. But for the two ball interaction in a bounded shear flow, we have applied the following approach developed in [40] to predict the ball positions: For the interaction during the two ball encounter, we have to impose a minimal gap of size $ch$ between the balls where $c$ is some constant between 0 and 1, $h$ being the mesh size of the velocity field. Then, when advancing the two ball mass centers, we proceed as follows at each sub-cycling time step: (i) we do nothing if the gap between the two balls at the new position is greater or equal than $ch$, (ii) if the gap size of the two balls at the new position is less than $ch$, we do not advance the balls directly; but instead we first move the ball centers in the direction perpendicularly to the line joining the previous centers, and then move them in the direction parallel to the line joining the previous centers, and make sure that the gap size is no less than $ch$. For all the simulations reported in this article, relying on this strategy, we took $h/16$ as minimal gap size.

In system (30)–(32), there are two multipliers: namely $p$ and $\lambda$. We have solved this system via an Uzawa-conjugate gradient method driven by both multipliers (an one shot method, similar to those discussed in, e.g., [19, 41, 42]). The general problem is as follows:

Find $u \in W_h$, $u = g_0$ on $\Gamma$, $p \in L^2_{0h}$, $\lambda \in \Lambda_h$, $V \in \mathbb{R}^3$, $\omega \in \mathbb{R}^3$ so that

$$
\begin{aligned}
-\int_\Omega p \nabla \cdot v dx + \mu \int_\Omega \nabla u : \nabla v dx + M_p \frac{V - V_0}{\Delta t} \cdot Y + \frac{I_p \omega - \omega_0}{\Delta t} \cdot \xi &= (1 - \frac{\rho_f}{\rho_s}) M_p g \cdot Y < \lambda, v - Y - \xi \times \nabla X >_{\Lambda_h} + \int_\Omega F \cdot v dx, \\
\forall v \in W_{0h}, Y \in \mathbb{R}^3, \xi \in \mathbb{R}^3,
\end{aligned}
$$

(36)

$$
\int_\Omega q \nabla \cdot u dx = 0, \forall q \in L^2_h,
$$

(37)

$$
< \mu, u - V - \omega \nabla X >_{\Lambda_h} = 0, \forall \mu \in \Lambda_h.
$$

(38)

To solve system (36)–(38) we employed the following Uzawa-conjugate gradient algorithm operating in the space $L^2_{0h} \times \Lambda_h$:
\( p^0 \in L^2_{\text{oh}} \) and \( \lambda^0 \in \Lambda_h \) are given; solve

\[
\begin{cases}
\mu \int_{\Omega} \nabla u^0 : \nabla v \, dx = \int_{\Omega} p^0 \nabla \cdot v \, dx + \langle \lambda^0, v \rangle_{\Lambda_h} + \int_{\Omega} F \cdot v \, dx, \\
\forall v \in W_{\text{oh}}, \ u^0 \in W_h, \ u = g_{\text{oh}} \text{ on } \Gamma,
\end{cases}
\]

\( M_p \frac{V^0 - V_0}{\Delta t} \cdot Y = (1 - \frac{\rho_f}{\rho_s}) M_p g \cdot Y - \langle \lambda^0, Y \rangle_{\Lambda_h}, \quad \forall Y \in \mathbb{R}^3, \quad (40) \)

\( I_p \frac{\omega^0 - \omega_0}{\Delta t} \cdot \xi = -\langle \lambda^0, \xi \times \overrightarrow{Gx} \rangle_{\Lambda_h}, \quad \forall \xi \in \mathbb{R}^3, \quad (41) \)

and then compute

\( g^0_1 = \nabla \cdot u^0; \quad (42) \)

next solve

\[
\begin{cases}
g^0_2 \in \Lambda_h, \\
\langle \mu, g^0_2 \rangle_{\Lambda_h} = \langle \mu, u^0 - V^0 - \omega^0 \times \overrightarrow{Gx} \rangle_{\Lambda_h}, \quad \forall \mu \in \Lambda_h,
\end{cases}
\]

and set

\( w_1^0 = g^0_1, \ w_2^0 = g^0_2. \quad (44) \)

Then for \( k \geq 0 \), assuming that \( p^k, \lambda^k, \ u^k, \ V^k, \omega^k, g^k_1, g^k_2, w^k_1 \) and \( w^k_2 \) are known, compute \( p^{k+1}, \lambda^{k+1}, \ u^{k+1}, \ V^{k+1}, \omega^{k+1}, g^{k+1}_1, g^{k+1}_2, w^{k+1}_1, w^{k+1}_2 \) as follows:

solve:

\[
\begin{cases}
\mu \int_{\Omega} \nabla \overline{u}^k : \nabla v \, dx = \int_{\Omega} w^k_1 \nabla \cdot v \, dx + \langle w^k_2, v \rangle_{\Lambda_h}, \\
\forall v \in W_{\text{oh}}, \ \overline{u}^k \in W_{\text{oh}},
\end{cases}
\]

\( M_p \frac{\overline{V}^k}{\Delta t} \cdot Y = -\langle w^k_2, Y \rangle_{\Lambda_h}, \quad \forall Y \in \mathbb{R}^3, \quad (46) \)

\( I_p \frac{\overline{\omega}^k}{\Delta t} \cdot \xi = -\langle w^k_2, \xi \times \overrightarrow{Gx} \rangle_{\Lambda_h}, \quad \forall \xi \in \mathbb{R}^3, \quad (47) \)

and then compute

\( \overline{g}^k_1 = \nabla \cdot \overline{u}^k; \quad (48) \)

next solve

\[
\begin{cases}
g^k_2 \in \Lambda_h, \\
\langle \mu, g^k_2 \rangle_{\Lambda_h} = \langle \mu, \overline{u}^k - \overline{\omega}^k \times \overrightarrow{Gx} \rangle_{\Lambda_h}, \quad \forall \mu \in \Lambda_h,
\end{cases}
\]

and compute

\[
\rho^k = \frac{\int_{\Omega} |g^k_1|^2 \, dx + \langle g^k_2, g^k_2 \rangle_{\Lambda_h}}{\int_{\Omega} \overline{g}^k_1 \overline{w}^k_1 \, dx + \langle g^k_2, w^k_2 \rangle_{\Lambda_h}}, \quad (50)
\]

\( \rho^k \) is then used to update the previous solution.\[12\]
and

\[\begin{align*}
    p^{k+1} &= p^k - \rho_k w_1^k, \\
    \lambda^{k+1} &= \lambda^k - \rho_k w_2^k, \\
    u^{k+1} &= u^k - \rho_k \bar{u}^k, \\
    V^{k+1} &= V^k - \rho_k \bar{V}^k, \\
    \omega^{k+1} &= \omega^k - \rho_k \bar{\omega}^k, \\
    g_1^{k+1} &= g_1^k - \rho_k \bar{g}_1^k, \\
    g_2^{k+1} &= g_2^k - \rho_k \bar{g}_2^k.
\end{align*}\]

(51) (52) (53) (54) (55) (56) (57)

If

\[\frac{\int_{\Omega} |g_1^{k+1}|^2 \, dx + < g_2^{k+1}, g_2^{k+1} >_{\Lambda_h}}{\int_{\Omega} |g_0|^2 \, dx + < g_2^0, g_2^0 >_{\Lambda_h}} \leq tol\]

(58)

take \( p = p^{k+1}, \lambda = \lambda^{k+1}, u = u^{k+1}, V = V^{k+1}, \omega = \omega^{k+1} \); else, compute

\[\gamma_k = \frac{\int_{\Omega} |g_1^{k+1}|^2 \, dx + < g_2^{k+1}, g_2^{k+1} >_{\Lambda_h}}{\int_{\Omega} |g_1|^2 \, dx + < g_2^0, g_2^0 >_{\Lambda_h}}\]

(59)

and set

\[\begin{align*}
    w_1^{k+1} &= g_1^{k+1} + \gamma_k w_1^k, \\
    w_2^{k+1} &= g_2^{k+1} + \gamma_k w_2^k.
\end{align*}\]

(60) (61)

Do \( k \leftarrow k + 1 \) and go back to (45).

In this article, we took \( tol = 10^{-14} \).

3 Numerical results

3.1 A ball rotating in a bounded shear flow

We have considered first the case of a neutrally buoyant ball which is suspended and freely moving in a Newtonian fluid. Its mass center is located at \((0, 0, 0)\) initially. The computational domain is \( \Omega = (-2, 2) \times (-2, 2) \times (-H/2, H/2) \) (i.e., \( L_1 = L_2 = 4 \)), the values of \( H \) being 0.75, 1, 1.5, 3, and 6. The ball radius \( a \) is 0.15, while the fluid and particle densities are \( \rho_f = \rho_s = 1 \), the fluid viscosity being \( \mu_f = 1 \). The confined ratio is defined as \( K = 2a/H \) where \( H \) is the distance between the two horizontal walls. The shear rate is fixed at \( \dot{\gamma} = 1 \) so that the velocity of the top wall (resp., bottom wall) is \( U = H/2 \) (resp., \( -U = -H/2 \)). The mesh size for the velocity field is either \( h = 1/32, 1/48, \) or 96, the mesh size for the pressure is \( 2h \), and the time
Figure 3: Snapshots of the velocity field projected on the $x_1x_3$-plane for $K = 0.2$ (top) and 0.3 (bottom).

Figure 4: The rotating speed versus the confined ratio (top) and the log–log plot of the difference of the rotation velocity versus the confined ratio (bottom). The solid line in the log–log plot shows the following power law effect of the confined ratio: $\omega = 0.5 - 0.22K^{2.935}$ for $0.1 \leq K \leq 0.4$. 
Figure 5: Comparison of the angular velocity of a single ball freely rotating in an Oldroyd-B fluid with its mass center fixed at (0,0,0) for different values of the Weissenberg number \(\text{Wi (}=\frac{\lambda_1}{\dot{\gamma}})\).

step is \(\Delta t = 0.001\). Under creeping flow conditions, the rotating velocity of the ball with respect to the \(x_2\)-axis is \(\dot{\gamma}/2 = 0.5\) in an unbounded shear flow according to the associated Jeffery’s solution [13]. Snapshots of the velocity field projected on the \(x_1x_3\)-plane for the cases \(K = 0.2\) and 0.3, computed with \(h = 1/96\), are shown in Fig. 3. The plot of the rotation speed versus the confined ratio being presented in Fig. 4. The computed angular speeds for \(K = 0.05\) and 0.1 are in a good agreement with Jeffery’s solution. The confined ratio affects the rotation speed as visualized in Fig. 4 where the solid line in the log–log plot shows for \(\omega\) a confined ratio power law dependence given (approximately) by \(\omega = 0.5 - 0.22K^{2.935}\) for \(0.1 \leq K \leq 0.4\). For all the numerical simulations considered in this article, we assume that all dimensional quantities are in the physical CGS units.

For the cases of a single ball freely rotating in an Oldroyd-B fluid with its mass center fixed at (0,0,0), we have considered different values of the relaxation time \(\lambda_1\). The ball radius \(a\) is 0.1, while the fluid and particle densities are \(\rho_f = \rho_s = 1\), the fluid viscosity being \(\mu_f = 1\). The computational domain is \(\Omega = (-1.5, 1.5) \times (-1.5, 1.5) \times (-1.5, 1.5)\). Then the blockage ratio is \(K = 1/15\) (same as the one used in [14]). The mesh size for the velocity field is \(h = 1/64\), the mesh size for the pressure is \(2h\), and the time step is \(\Delta t = 0.001\). The rotating velocities reported in Fig. 5 are in a good agreement with those reported in [14]. We have also considered different values of the retardation times, namely \(\lambda_2 = \lambda_1/\beta\) with \(\beta = 1.7, 1.8, 2, 4, \text{ and } 8\). Our numerical results shown in Fig. 5 suggest that the retardation time affects also the rotating speed. The reasonable range of the value of \(\beta = \frac{\lambda_1}{\lambda_2}\) is about between 1.7 and 2 when comparing with the experimental results of the rotating velocity in a Boger fluid reported in [44].
\[ \Delta s - U \Gamma \]

Figure 6: Two balls interacting in a bounded shear flow.

\[ -0.5 -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5 \]

\[ D=1.0 \quad D=0.5 \quad D=0.316 \quad D=0.255 \quad D=0.194 \quad D=0.122 \]

Figure 7: Projected trajectories of the two ball mass centers in a bounded shear flow for \( Wi=0 \) where the higher ball (initially located above \( x_3 = 0 \) and at \( x_1 = -0.5 \)) moves from the left to the right and the lower ball (initially located below \( x_3 = 0 \) and at \( x_1 = 0.5 \)) moves from the right to the left: (a) the balls pass over/under for \( D =1.0, 05, \) and \( 0.316, \) and (b) the balls swap for \( D =0.255, 0.194, \) and \( 0.122. \)

### 3.2 Two balls interacting in a two wall driven bounded shear flow

In this section we consider the case of two balls of the same size interacting in a bounded shear flow as visualized in Fig. 6. The ball radii are \( a = 0.1. \) The fluid and ball densities are \( \rho_f = \rho_s = 1, \) the viscosity being \( \mu = 1. \) The relaxation time \( \lambda_1 \) takes the values \( 0.1, 0.25, 0.5, 0.75 \) and \( 1, \) the retardation time being \( \lambda_2 = \lambda_1/8. \) The computational domain is \( \Omega = (-1.5, 1.5) \times (-1, 1) \times (-0.5, 0.5) \) (i.e., \( L_1 = 3 \) and \( L_2 = 2. \)) The shear rate is fixed at \( \dot{\gamma} = 1 \) so the velocity of the top wall is \( U = 0.5, \) the bottom wall velocity being \( U = -0.5. \) The mass centers of the two balls are located on the shear plane at \( (-d_0, 0, \Delta s) \) and \( (d_0, 0, -\Delta s) \) initially, where \( \Delta s \) varies and \( d_0 \) is 0.5. The mesh size for the velocity field and the conformation tensor is \( h = 1/48, \) the mesh size for the pressure is \( 2h, \) the time step being \( \Delta t = 0.001. \)
Figure 8: Projected trajectories of the two ball mass centers in a bounded shear flow for \( Wi=0.1 \) where the higher ball (initially located above \( x_3 = 0 \) and at \( x_1 = -0.5 \)) moves from the left to the right and the lower ball (initially located below \( x_3 = 0 \) and at \( x_1 = 0.5 \)) moves from the right to the left: (a) the balls pass over/under for \( D = 0.1 \) and 0.5, (b) the balls swap for \( D = 0.255, 0.194 \) and 0.122, and (c) the balls chain and then tumble for \( D =0.316 \) and 0.42.

Figure 9: Projected trajectories of the two ball mass centers in a bounded shear flow for \( Wi=0.25 \) where the higher ball (initially located above \( x_3 = 0 \) and at \( x_1 = -0.5 \)) moves from the left to the right and the lower ball (initially located below \( x_3 = 0 \) and at \( x_1 = 0.5 \)) moves from the right to the left: (a) the balls pass over/under for \( D = 0.1 \) and 0.5, (b) the balls swap for \( D = 0.255, 0.194 \) and 0.122, and (c) the balls chain and tumble for \( D = 0.316 \) and 0.42.
Figure 10: Projected trajectories of the two ball mass centers in a bounded shear flow for Wi=0.5 where the higher ball (initially located above $x_3 = 0$ and at $x_1 = -0.5$) moves from the left to the right and the lower ball (initially located below $x_3 = 0$ and at $x_1 = 0.5$) moves from the right to the left: (a) the balls pass over/under for $D = 0.1$ and 0.5, (b) the balls swap for $D = 0.194$ and 0.122, and (c) the balls chain and tumble for $D = 0.255, 0.316$ and 0.42.

Figure 11: Projected trajectories of the two ball mass centers in a bounded shear flow for Wi=0.75 where the higher ball (initially located above $x_3 = 0$ and at $x_1 = -0.5$) moves from the left to the right and the lower ball (initially located below $x_3 = 0$ and at $x_1 = 0.5$) moves from the right to the left: (a) the balls pass over/under for $D = 0.1, 0.5$ and 0.42, (b) the balls swap for $D = 0.194$ and 0.122, and (c) the balls tumble and then kayak for $D = 0.255$ and 0.316.
Figure 12: Projected trajectories of the two ball mass centers in a bounded shear flow for $Wi=1$ where the higher ball (initially located above $x_3 = 0$ and at $x_1 = -0.5$) moves from the left to the right and the lower ball (initially located below $x_3 = 0$ and at $x_1 = 0.5$) moves from the right to the left: (a) the balls pass over/under for $D = 0.1, 0.5$ and $0.38$ (b) the balls swap for $D = 0.122$, and (c) the balls tumble and then kayak for $D = 0.194, 0.255$ and $0.316$.

The dimensionless initial vertical displacements from the ball center to the middle plane, namely $D = \Delta s/a$, are indicated in Figs 7 to 12. The Weissenberg number is $Wi=\dot{\gamma} \lambda_1$.

When two balls move in a bounded shear flow of a Newtonian fluid at Stokes regime, the higher ball takes over the lower one and then both return to their initial heights for those large vertical displacements $D = 0.316, 0.5$ and $1$ as in Fig. 7. These two particle paths are called pass (or open) trajectories. But for smaller vertical displacements, $D = 0.122, 0.255$ and $0.316$, they first come close to each other and to the mid-plane between the two horizontal walls, then, the balls move away from each other and from the above mid-plane. These paths of the two particle are called return trajectories. Both kinds are on the shear plane as shown in Fig. 7 for $Wi=0$ (Newtonian case) and they are consistent with the results obtained in [3].

For the two balls interacting in an Oldroyd-B fluid with the same setup and initial position, we have summarized the results for $Wi=0.1, 0.25, 0.5, 0.75$, and $1$ in Figs. 8 to 12. As in Newtonian fluids, there are results of pass and return trajectories concerning two ball encounters; but the trajectories of the two ball mass centers lose the symmetry due to the effect of elastic force arising from viscoelastic fluids. For example, the open trajectories associated with $D = 0.5$ for $Wi=0.1, 0.25, 0.5$, and $1$ are closer to the mid-plane after the two balls pass over/under each other. The elastic force is not strong enough to hold them together during passing over/under, but it already pulls the balls toward each other and then changes the shape of the
Figure 13: Phase diagram for the motion of two balls based on the initial vertical displacement $D$ and on the Weissenberg number $Wi$ in a bounded shear flow.

Figure 14: The ball position of the kayaking motion viewed in the $x_1$—direction for $Wi=1$ and $D = 0.255$ at $t = 69, 71, 80, 81, 83, 88, 90, 92,$ and $93$ (from left to right and top to bottom): the kayaking motion of the two ball mass centers is rotating about the $x_2$—direction.
trajectories. Thus the trajectories lose their symmetry. For the higher values of \( Wi \) considered in this section, there are less return trajectories; instead it is easier to obtain the chain of two balls once they run into each other. Actually depending on the Weissenberg number \( Wi \) and on the initial vertical displacement \( \Delta s \), two balls can form a chain in a bounded shear flow, and then such chain tumbles. For example, for \( D = 0.316 \), the two balls come close to each other, form a chain and then rotate with respect to the midpoint between two mass centers (i.e., they tumble) for \( Wi=0.1, 0.25, 0.5, \) and \( 1 \). The distance between two balls in the \( x_1 \)-direction becomes bigger for higher value of \( Wi \). The details of the phase diagram of pass, return, and tumbling are shown in Fig. 13. The range of the vertical distance for the passing over becomes bigger for higher Weissenberg numbers. For the shear flows considered in this article, increasing the \( Wi \) with a fixed shear rate is equivalent to increase the shear rate with a fixed relaxation time. This explains why, for \( Wi=1 \), two balls can have a bigger gap between them while rotating with respect to the middle point between the two mass centers since the two balls are kind of moving under higher shear rate. Those trajectories of the tumbling motion are similar to the closed streamlines around a freely rotating ball centered at the origin shown in Figs. 8 to 10.

For both higher values, \( Wi=0.75 \) and \( 1 \), the tumbling motion can change to kayaking motion later on as shown in, e.g., Fig. 14 for \( Wi=1 \) and \( D = 0.255 \). The chain of two balls can be viewed as a long body, even though they are not rigidly connected. For a rigid long body rotating in a bounded shear flow of a Newtonian fluid, its stable motion is its long axis tumbling in the shear plane (i.e., the \( x_1x_3 \)-plane) due to the effect of the particle inertia (e.g., see [45]). Thus for the cases of lower values of \( Wi \) considered above, i.e., \( Wi=0.1, 0.25 \) and \( 0.5 \), the tumbling motion of two balls in the shear plane is consistent with the stable motion of the long body in a Newtonian fluid. For \( Wi=0.75 \) and \( 1 \), those numerical results of the kayaking motion suggest that for a rigid long body rotating in a bounded shear flow of an Oldroyd-B fluid, its long axis migrates out of the shear plane. Those numerical results do not conflict with those of an ellipsoid in a bounded shear flow of a Giesekus fluid obtained by D’Avino et al. in [46] and [47] since they did not include the effect of the particle and fluid inertia in their simulations.

4 Conclusions

In this article, we discussed a new distributed Lagrange multiplier/fictitious domain method for simulating fluid-particle interaction in three-dimensional Stokes flow of Oldroyd-B fluids. The methodology is validated by comparing the numerical results associated with a neutrally buoyant ball. For the cases of two ball encounters under creeping flow conditions in a bounded shear flow for the Weisenberg number \( Wi \) up to \( 1 \), the trajectories of the two ball mass centers are either passing over/under or returning if they don’t chain. If the two balls form a chain, they tumble in the
shear plane for the lower values of the Weissenberg number. But for higher values of Wi, they can tumble first and then kayak later. Those numerical results for two ball chains suggest that it is worth to further study the effect of the particle inertia on the orientation of an ellipsoid in a bounded shear flow of either Oldroyd-B or Giesekus types.

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