

A Distributed Lagrange Multiplier/Fictitious Domain Method for Viscoelastic Particulate Flows

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A distributed Lagrange multiplier/fictitious domain method (DLM) is developed for simulating the motion of rigid particles suspended in the Oldroyd-B fluid. This method is a generalization of the one described in [1] where the motion of particles suspended in a Newtonian fluid was simulated. In our implementation of the DLM method, the fluid-particle system is treated implicitly using a combined weak formulation in which the forces and moments between the particles and fluid cancel. The governing equations for the Oldroyd-B liquid are solved everywhere, including inside the particles. The flow inside the particles is forced to be a rigid body motion by a distribution of Lagrange multipliers. We use the Marchuk-Yanenko operator-splitting technique to decouple the difficulties associated with the incompressibility constraint, nonlinear convection and viscoelastic terms. The constitutive equation is solved using a scheme that guarantees the positive definiteness of the configuration tensor while the convection term in the constitutive equation is discretized using a third order upwinding scheme. The nonlinear convection problem is solved using a least square conjugate gradient algorithm, and the Stokes like problem is solved using a conjugate gradient algorithm. The code is verified performing a convergence study to show that the results are independent of the mesh and time step sizes. Our simulations show that when particles are dropped in a channel, and the viscoelastic Mach number (M) is less than one and the elasticity number (E) is greater than one, the particles chain along the flow direction; this agrees with the results presented in [2]. In our simulations of the fluidization of 102 particles in a two dimensional bed we find that the particles near the channel walls form chains that are parallel to the walls, but the distribution of particles away from the walls is relatively random.

1. Introduction

The capability of numerically simulating the motion of particles suspended in Newtonian and viscoelastic fluids could be useful in many applications, e.g., for developing theoretical models of particulate systems which in turn could be useful for improving particle handling devices.

Our goal in this paper is to extend the distributed Lagrange multiplier/fictitious domain method presented in [1] to simulate the motion of rigid particles suspended in a viscoelastic (Oldroyd-B) fluid; this method is used to study the motion, and interactions, of rigid particles. It is well known that when an ellipse, or a long particle, is dropped in a Newtonian liquid it falls with its broad side normal to the falling direction. In a viscoelastic liquid, on the other hand, the ellipse falls with its broad side parallel to the falling direction. It was recently shown in [2,3] that the orientation of the particle depends on the relative importance of the inertia and viscoelastic stresses. In particular, the inertia tends to turn a long body broad side on and the elastic stresses tend to do the opposite. It is, in fact, possible to have a regime where these two stresses are of the same order. In this regime a long body may fall with its broad side at an angle to the direction of fall, but the tilted equilibrium is unstable.

A similar result holds for the relative orientation of two or more particles falling in a viscoelastic liquid. Specifically, the particles align such that the line joining their centers is approximately parallel to the falling direction [3]. The same mechanism is important when a dilute suspension containing a random distribution of solid particles is subjected to a simple shear flow. The viscoelastic stresses cause the particles to align in the direction parallel to the flow. In other words, the viscoelastic and inertial stresses, depending on their relative magnitudes, may lead to the formation of different configurations, or microstructures, at the particle length scales. An understanding of the mechanisms that may lead to the formation of these particle scale microstructures is important because they determine the macroscopic transport properties of the composite fluid.

The interaction of particles in an Oldroyd-B fluid was first simulated in [2,4-6] by using the arbitrary Eulerian Lagrangian approach. The authors successfully simulated the motion of several particles in a two dimensional channel. These simulations reproduced the qualitative features of the motion of particles in a fluidized suspension, i.e., the particles form chains in the direction parallel to the flow. These authors have also shown that when a critical Mach number is less than one and an elasticity number is greater than one an ellipse sedimenting in the Oldroyd-B fluid falls with its largest axis parallel to the flow.

As noted before, the DLM method implemented in this paper for viscoelastic liquids is an extension of the method developed in [1,7] for Newtonian fluids. One of the key features of the method is that the fluid-particle system is treated implicitly by using a combined weak formulation where the forces and moments between the particles and fluid cancel, as they are internal to the

combined system. These internal hydrodynamic forces are not needed for determining the motion of particles. In our combined weak formulation we solve fluid flow equations everywhere in the domain, including inside the particles. The flow inside the particles is forced to be a rigid body motion using the distributed Lagrange multiplier method. This multiplier represents the additional body force per unit volume needed to maintain rigid-body motion inside the particle boundary, and is analogous to the pressure in incompressible fluid flow, whose gradient is the force needed to maintain the constraint of incompressibility.

In our numerical method the Marchuk-Yanenko operator splitting technique is used to decouple the difficulties associated with the incompressibility constraint, the nonlinear convection term, the viscoelastic term and the rigid body motion constraint. This gives rise to the four sub-problems that are solved using matrix-free algorithms. The code is verified by comparing the time dependent velocity and configuration (stress) distributions for a circular particle falling in a channel for two different mesh refinements, and for two different time steps. It is shown that the results are independent of the mesh resolution and the time step.

It was discussed in [2] and [3] that when two or more particles are dropped in a channel the orientation of particles relative to the direction of flow is determined by the Mach number $M = \sqrt{\text{Re} \text{De}}$ and the elasticity number $E = \frac{\text{De}}{\text{Re}}$. Here $\text{De} = \frac{U\lambda_r}{D}$ is the Deborah number, and $\text{Re} = \frac{\rho_L U D}{\eta}$ is the Reynolds number, where λ_r is the relaxation time of the fluid, η is the zero shear viscosity of the fluid, U is the particle velocity, and D is the particle diameter. In [2] it was shown that when M is less than one and E is greater than one, the particles align themselves parallel to the flow direction.

The same results arise in our simulations; two sedimenting particles align parallel to the direction of flow when $M < 1$ and $E > 1$ and eleven particles dropped in a channel formed two or more groups and within each group the particles formed chains that were parallel to the flow. But, when the two conditions $M < 1$ and $E > 1$ are not satisfied the particles do not sediment by aligning parallel to the direction of flow. Our simulations show that the viscoelastic stresses are important in determining the relative orientation of sedimenting particles. In our simulations of the fluidization of 102 particles in a bed we find that the particles form chains along the channel walls. Away from the walls, however, the relative orientation of particles is far less organized.

2. Problem statement and numerical method

The viscoelastic fluid is modeled via the Oldroyd-B model. In this paper we will present results for two-dimensional flows. The results for the three-dimensional case will be discussed in a

future paper. In our simulations we will assume that the lubrication forces are large enough to prevent the particles from touching each other or the walls. This is enforced by applying a body force to the particles when the distance between two particles, or between a particle and a wall, is of the order of the element size.

Let us denote the domain containing the viscoelastic fluid and N particles by Ω , and the interior of the i th particle by $P_i(t)$. For simplicity we will assume that the domain is rectangular with boundary Γ . The four sides of the domain will be denoted by $\Gamma_1, \Gamma_2, \Gamma_3$, and Γ_4 (see Figure 1), and Γ^- will be used to denote the upstream part of Γ . The governing equations for the fluid-particle system are:

$$\rho_L \left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = \rho_L \mathbf{g} - \nabla p + \nabla \cdot \left(\frac{c}{\lambda_r} \mathbf{A} \right) + \nabla \cdot (2\eta_s \mathbf{D}) \quad \text{in } \Omega \setminus \overline{P(t)} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \setminus \overline{P(t)} \quad (2)$$

$$\mathbf{u} = \mathbf{u}_L \quad \text{on } \Gamma \quad (3)$$

$$\mathbf{u} = \mathbf{U}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i \quad \text{on } \partial P_i(t), i=1, \dots, N, \quad (4)$$

with the evolution of the configuration tensor \mathbf{A} given by

$$\frac{\partial \mathbf{A}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{A} = \mathbf{A} \cdot \nabla \mathbf{u} + \nabla \mathbf{u}^T \cdot \mathbf{A} - \frac{1}{\lambda_r} (\mathbf{A} - \mathbf{I}), \quad (5)$$

$$\mathbf{A} = \mathbf{A}_L \quad \text{on } \Gamma^-.$$

Here \mathbf{u} is the velocity, p is the pressure, η_s is the solvent viscosity, ρ_L is the density, \mathbf{D} is the symmetric part of the velocity gradient tensor, c is a measure of polymer concentration in terms of the zero shear viscosity, and where λ_r is the relaxation time. The zero shear viscosity $\eta = \eta_s + \eta_p$, where $\eta_p = c \eta_s$ is the polymer contribution to viscosity. The fluid retardation time is equal to $\frac{\lambda_r}{1+c}$. The above

equations are solved with the following initial conditions:

$$\mathbf{u} |_{t=0} = \mathbf{u}_0 \quad (6)$$

$$\mathbf{A} |_{t=0} = \mathbf{A}_0 \quad (7)$$

where \mathbf{u}_0 and \mathbf{A}_0 are the known initial values of the velocity and the configuration tensor.

The particle velocity \mathbf{U}_i and angular velocity $\boldsymbol{\omega}_i$ are governed by

$$M_i \frac{d\mathbf{U}_i}{dt} = M_i \mathbf{g} + \mathbf{F}_i \quad (8)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \mathbf{T}_i \quad (9)$$

$$\mathbf{U}_i |_{t=0} = \mathbf{U}_{i,0} \quad (10)$$

$$\boldsymbol{\omega}_i |_{t=0} = \boldsymbol{\omega}_{i,0} \quad (11)$$

where M_i and I_i are the mass and moment of inertia of the i th particle, and \mathbf{F}_i and \mathbf{T}_i are the force and torque acting on the i th particle. In this investigation we will assume that the particles are circular, and therefore we do not need to keep track of the particle orientation. The particle positions are obtained from

$$\frac{d\mathbf{X}_i}{dt} = \mathbf{U}_i \quad (12)$$

$$\mathbf{X}_i |_{t=0} = \mathbf{X}_{i,0} \quad (13)$$

where $\mathbf{X}_{i,0}$ is the position of the i th particle at time $t=0$.

2.1 Collision strategy

The collisions among the particles, and the particles and the domain walls, are prevented by applying a body force that acts when the distance between two particles, or between a particle and a wall, is of the order of the element size. This additional body force--which is repulsive in nature--is added to equation (8). The particle-particle repulsive force is given by

$$\mathbf{F}_{ij}^p = \begin{cases} 0 & \text{for } d_{i,j} > R_i + R_j + \rho \\ \frac{1}{\epsilon_p} (\mathbf{X}_i - \mathbf{X}_j) (R_i + R_j + \rho - d_{i,j})^2, & \text{for } d_{i,j} < R_i + R_j + \rho \end{cases} \quad (14)$$

where $d_{i,j}$ is the distance between the centers of the i th and j th particles, R_i is radius of the i th particle and ρ is the force range, and ϵ_p is a small positive stiffness parameter. The repulsive force between the particles and the wall is given by

$$\mathbf{F}_{ij}^w = \begin{cases} 0 & \text{for } d_i > 2R_i + \rho \\ \frac{1}{\epsilon_w} (\mathbf{X}_i - \mathbf{X}_j) (2R_i + \rho - d_i)^2, & \text{for } d_i < 2R_i + \rho \end{cases} \quad (15)$$

where d_i is the distance between the centers of the i th particle and the imaginary particle on the other side of the wall Γ_j , and ϵ_w is another small positive stiffness parameter (see Figure 2). The above particle-particle repulsive forces and the particle-wall repulsive forces are added to equation to obtain

$$M_i \frac{d\mathbf{U}_i}{dt} = M_i \mathbf{g} + \mathbf{F}_i + \mathbf{F}'_i$$

where

$$\mathbf{F}'_i = \sum_{\substack{j=1 \\ j \neq i}}^N \mathbf{F}_{i,j}^P + \sum_{j=1}^4 \mathbf{F}_{i,j}^W$$

is the repulsive force exerted on the i th particle by the other particles and the walls. In our simulations, ρ is equal to one and half times the velocity mesh size, $\varepsilon_w = 10^{-5}$ and $\varepsilon_p = 2\varepsilon_w$. The repulsive force acts only when the distance between the particles is smaller than ρ .

2.2 Weak form

The approach used in [1,7] is followed for obtaining the weak form of the governing equations stated in the previous section. The only additional complication being that the fluid is viscoelastic, and thus we also need to solve the constitutive equation (5) along with the other equations. In obtaining this weak form, the hydrodynamic forces and torques acting on the particles can be completely eliminated by combining the fluid and particle equations of motion into a single weak equation of motion for the combined fluid-particle system. This total momentum equation for the fluid-particle systems was first introduced in [8]. For simplicity, we will assume that there is only one particle. The extension to the many-particle case is straightforward.

To state the combined weak form for the equation of motion we need the following two spaces:

$$\begin{aligned} \overline{V}_{u\Gamma}(t) &= \{(\mathbf{v}, \mathbf{V}, \xi) \mid \mathbf{v} \in H^1(\Omega)^2, \mathbf{V} \in \mathbf{R}^2, \xi \in \mathbf{R}, \mathbf{v} = \mathbf{V} + \xi \times \mathbf{r} \text{ in } P(t), \text{ and } \mathbf{v} = \mathbf{u}_\Gamma(t) \text{ on } \Gamma\}, \\ \overline{V}_0(t) &= \{(\mathbf{v}, \mathbf{V}, \xi) \mid \mathbf{v} \in H^1(\Omega)^2, \mathbf{V} \in \mathbf{R}^2, \xi \in \mathbf{R}, \mathbf{v} = \mathbf{V} + \xi \times \mathbf{r} \text{ in } P(t), \text{ and } \mathbf{v} = 0 \text{ on } \Gamma\}, \end{aligned} \quad (16)$$

where \mathbf{R} denotes the set of real numbers. The extended fluid-particle velocity $(\mathbf{u}, \mathbf{U}, \omega)$ lie in $\overline{V}_{u\Gamma}$, and the equation of motion in Ω is

$$\begin{aligned} \int_{\Omega} \rho_L \left(\frac{d\mathbf{u}}{dt} - \mathbf{g} \right) \cdot \mathbf{v} dx + \left(1 - \frac{\rho_L}{\rho_d} \right) \left(\int_{\Omega} \left(\mathbf{M} \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + \mathbf{I} \frac{d\omega}{dt} \xi \right) - \mathbf{F}' \cdot \mathbf{V} = \int_{\Omega} \boldsymbol{\sigma} : \mathbf{D}[\mathbf{v}] dx, \right. \\ \left. \text{for all } (\mathbf{v}, \mathbf{V}, \xi) \in \overline{V}_0, \right. \end{aligned}$$

where $\boldsymbol{\sigma} = -p \mathbf{I} + \frac{c}{\lambda_r} \mathbf{A} + 2\eta_s \mathbf{D}$ is the stress tensor.

In the above equation the solution \mathbf{u} and variation \mathbf{v} are required to satisfy the strong form of the constraint of rigid body motion throughout $P(t)$. In the distributed Lagrange multiplier method this constraint is removed from the velocity space and enforced weakly as a side constraint using a distributed Lagrange multiplier term. It was shown in [1,7] that the following weak formulation of the problem holds in the extended domain:

For a.e. $t > 0$, find $\mathbf{u} \in \overline{W}_{u\Gamma}$, $\mathbf{A} \in \overline{W}_A$, $p \in L^2_0(\Omega)$, $\boldsymbol{\lambda} \in \Lambda(t)$, $\mathbf{U} \in \mathbf{R}^2$, and $\omega \in \mathbf{R}$, satisfying

$$\begin{aligned} & \int_{\Omega} \rho_L \left(\frac{d\mathbf{u}}{dt} - \mathbf{g} \right) \cdot \mathbf{v} d\mathbf{x} - \int_{\Omega} p \nabla \cdot \mathbf{v} d\mathbf{x} + \int_{\Omega} 2\eta_s \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} - \int_{\Omega} \mathbf{v} \cdot \nabla \cdot \left(\frac{c}{\lambda_r} \mathbf{A} \right) d\mathbf{x} \\ & + \left(1 - \frac{\rho_L}{\rho_d} \right) \left(\mathbf{M} \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + I \frac{d\omega}{dt} \xi \right) - \mathbf{F}' \cdot \mathbf{V} = \langle \boldsymbol{\lambda}, \mathbf{v} - (\mathbf{V} + \xi \times \mathbf{r}) \rangle_{P(t)} \end{aligned}$$

for all $\mathbf{v} \in \overline{W}_0$, $\mathbf{V} \in \mathbf{R}^2$, and $\xi \in \mathbf{R}$, (17)

$$\int_{\Omega} q \nabla \cdot \mathbf{u} d\mathbf{x} = 0 \quad \text{for all } q \in L^2(\Omega), \quad (18)$$

$$\langle \boldsymbol{\mu}, \mathbf{u} - (\mathbf{U} + \omega \times \mathbf{r}) \rangle_{P(t)} = 0 \quad \text{for all } \boldsymbol{\mu} \in \Lambda(t), \quad (19)$$

$$\int_{\Omega} \left(\frac{\partial \mathbf{A}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{A} - \mathbf{A} \cdot \nabla \mathbf{u} - \nabla \mathbf{u}^T \cdot \mathbf{A} + \frac{1}{\lambda_r} (\mathbf{A} - \mathbf{I}) \right) \cdot \mathbf{s} d\mathbf{x} = 0 \quad \text{for all } \mathbf{s} \in \overline{W}_{A0}, \quad (20)$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_0 \quad \text{in } \Omega, \quad (21)$$

$$\mathbf{A}|_{t=0} = \mathbf{A}_0 \quad \text{in } \Omega, \quad (22)$$

as well as the kinematic equations and the initial conditions for the particle linear and angular velocities. Here

$$\begin{aligned} \overline{W}_{u\Gamma} &= \{ \mathbf{v} \in H^1(\Omega)^2 \mid \mathbf{v} = \mathbf{u}_{\Gamma}(t) \text{ on } \Gamma \}, \\ \overline{W}_0 &= H_0^1(\Omega)^2, \\ \overline{W}_A &= \{ \mathbf{A} \in H^1(\Omega)^3 \mid \mathbf{A} = \mathbf{A}_L(t) \text{ on } \Gamma^- \}, \\ \overline{W}_{A0} &= \{ \mathbf{A} \in H^1(\Omega)^3 \mid \mathbf{A} = \mathbf{0} \text{ on } \Gamma^- \}, \\ L_0^2(\Omega) &= \{ q \in L^2(\Omega) \mid \int_{\Omega} q d\mathbf{x} = 0 \} \end{aligned} \quad (23)$$

and $\Lambda(t)$ is $H^1(P(t))^2$, with $\langle \cdot, \cdot \rangle_{P(t)}$ denoting the H^1 inner product over the particle, where Γ^- is the upstream part of Γ . In our simulations, since the velocity and $\boldsymbol{\mu}$ are in H^1 , we will use the following H^1 inner product

$$\langle \boldsymbol{\mu}, \mathbf{v} \rangle_{P(t)} = \int_{P(t)} (\boldsymbol{\mu} \cdot \mathbf{v} + R^2 \nabla \boldsymbol{\mu} : \nabla \mathbf{v}) d\mathbf{x}, \quad (24)$$

where R is the particle radius.

2.3 Strong form

The strong form for the weak formulation of (17-22) can be obtained by integrating the stress term by parts. The resulting equations inside the region occupied by the fluid $\Omega \setminus \overline{P(t)}$ are

$$\begin{aligned} \rho_L \left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] &= \rho_L \mathbf{g} - \nabla p + \nabla \cdot \left(\frac{c}{\lambda_r} \mathbf{A} \right) + \nabla \cdot (2\eta_s \mathbf{D}), \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathbf{A}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{A} &= \mathbf{A} \cdot \nabla \mathbf{u} + \nabla \mathbf{u}^\top \cdot \mathbf{A} - \frac{1}{\lambda_r} (\mathbf{A} - \mathbf{I}), \\
\mathbf{u} &= \mathbf{u}_L && \text{on } \Gamma, \\
\mathbf{u} &= \mathbf{U}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i && \text{on } \partial P_i(t), i=1, \dots, N, \\
\mathbf{A} &= \mathbf{A}_L && \text{on } \Gamma^-, \tag{25}
\end{aligned}$$

and the equations inside the region occupied by the particles $P(t)$ are

$$\begin{aligned}
\rho_L \left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] &= \rho_L \mathbf{g} - \nabla p + \nabla \cdot (2\eta_s \mathbf{D}) + \boldsymbol{\lambda} - R^2 \nabla^2 \boldsymbol{\lambda} \\
\mathbf{u} &= \mathbf{U}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i && \text{on } \partial P_i(t), i=1, \dots, N, \tag{26}
\end{aligned}$$

Here we have used the fact that the rigid body motion satisfies the incompressibility constraint and that the viscoelastic stress inside the particles is zero. The boundary condition on the interface between the fluid and particle regions $\partial P(t)$ is

$$\mathbf{n} \cdot (-\boldsymbol{\sigma}_L) = \mathbf{n} \cdot \nabla \boldsymbol{\lambda} \tag{27}$$

where \mathbf{n} is the normal at the fluid-particle interface, and $\boldsymbol{\sigma}_L = -p\mathbf{I} + 2\eta_s \mathbf{D} + \frac{c}{\lambda_r} \mathbf{A}$ is the stress in the fluid phase, and $\boldsymbol{\sigma}_p = 0$ is the stress inside the particles. For given $\mathbf{U}(t)$ and $\boldsymbol{\omega}(t)$, and the positions $X_i(t)$, $i=1, \dots, N$, equation (26) can be written as:

$$\boldsymbol{\lambda} - R^2 \nabla^2 \boldsymbol{\lambda} = \rho_L \left(\frac{d\mathbf{U}}{dt} + \frac{d\boldsymbol{\omega}}{dt} \times \mathbf{r} + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) - \mathbf{g} \right) \tag{28}$$

3. Finite-element approximation

In order to solve the above problem numerically, we will discretize the domain using a regular finite element triangulation T_h for the velocity and configuration tensor, where h is the mesh size, and a regular triangulation T_{2h} for the pressure. The following finite dimensional spaces are defined for approximating $\overline{W}_{u\Gamma}$, \overline{W}_0 , \overline{W}_A , \overline{W}_{A0} , $L^2(\Omega)$ and $L^2_0(\Omega)$:

$$\begin{aligned}
W_{u\Gamma,h} &= \{ \mathbf{v}_h \in C^0(\overline{\Omega})^2 \mid \mathbf{v}_h|_T \in P_1 \times P_1 \text{ for all } T \in T_h, \mathbf{v}_h = \mathbf{u}_{\Gamma,h} \text{ on } \Gamma \} \\
W_{0,h} &= \{ \mathbf{v}_h \in C^0(\overline{\Omega})^2 \mid \mathbf{v}_h|_T \in P_1 \times P_1 \text{ for all } T \in T_h, \mathbf{v}_h = 0 \text{ on } \Gamma \} \tag{29}
\end{aligned}$$

$$\begin{aligned}
L_h^2 &= \{ q_h \in C^0(\overline{\Omega}) \mid q_h|_T \in P_1 \text{ for all } T \in T_{2h} \} \\
L_{0,h}^2 &= \{ q_h \in L_h^2 \mid \int_{\Omega} q_h \, d\mathbf{x} = 0 \} \tag{30}
\end{aligned}$$

$$W_{A,h} = \{ \mathbf{s}_h \in C^0(\overline{\Omega})^3 \mid \mathbf{s}_h|_T \in P_1 \times P_1 \times P_1 \text{ for all } T \in T_h, \mathbf{s}_h = \mathbf{A}_{L,h} \text{ on } \Gamma^- \}$$

$$W_{A_{0,h}} = \{s_h \in C^0(\overline{\Omega})^3 \mid s_h|_T \in P_1 \times P_1 \times P_1 \text{ for all } T \in T_h, s_h = 0 \text{ on } \Gamma^-\} \quad (31)$$

where Γ^- is the upstream part of Γ . Using these finite dimensional spaces, the following finite-element approximation to the problem (17)-(22) is obtained:

Find $\mathbf{u}_h \in W_{u\Gamma,h}$, $\mathbf{A}_h \in W_{A,h}$, $p_h \in L^2_{0,h}$, $\boldsymbol{\lambda}_h \in \Lambda_h(t)$, $\mathbf{U} \in \mathbf{R}^2$, and $\boldsymbol{\omega} \in \mathbf{R}$, satisfying

$$\begin{aligned} & \int_{\Omega} \rho_L \left(\frac{d\mathbf{u}_h}{dt} - \mathbf{g} \right) \cdot \mathbf{v}_h \, dx - \int_{\Omega} p_h \nabla \cdot \mathbf{v}_h \, dx + \int_{\Omega} 2\eta_s \mathbf{D}[\mathbf{u}_h] : \mathbf{D}[\mathbf{v}_h] \, dx - \int_{\Omega} \mathbf{v}_h \cdot \nabla \cdot \left(\frac{c}{\lambda_r} \mathbf{A}_h \right) \, dx \\ & + \left(1 - \frac{\rho_L}{\rho_d} \right) \left(\mathbf{M} \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + \mathbf{I} \frac{d\boldsymbol{\omega}}{dt} \cdot \boldsymbol{\xi} \right) - \mathbf{F}' \cdot \mathbf{V} = \langle \boldsymbol{\lambda}_h, \mathbf{v}_h - (\mathbf{V} + \boldsymbol{\xi} \times \mathbf{r}) \rangle_{P(t)} \end{aligned}$$

for all $\mathbf{v}_h \in W_{0,h}$, $\mathbf{V} \in \mathbf{R}^2$, and $\boldsymbol{\xi} \in \mathbf{R}$,

$$\int_{\Omega} q_h \nabla \cdot \mathbf{u}_h \, dx = 0 \quad \text{for all } q_h \in L^2_h,$$

$$\langle \boldsymbol{\mu}_h, \mathbf{u}_h - (\mathbf{U} + \boldsymbol{\omega} \times \mathbf{r}) \rangle_{P(t)} = 0 \quad \text{for all } \boldsymbol{\mu}_h \in \Lambda_h(t),$$

$$\int_{\Omega} \left(\frac{\partial \mathbf{A}_h}{\partial t} + \mathbf{u}_h \cdot \nabla \mathbf{A}_h - \mathbf{A}_h \cdot \nabla \mathbf{u}_h - \nabla \mathbf{u}_h^T \cdot \mathbf{A}_h + \frac{1}{\lambda_r} (\mathbf{A}_h - \mathbf{I}) \cdot \mathbf{s}_h \right) \, dx = 0$$

for all $\mathbf{s}_h \in W_{A_{0,h}}$, and $\mathbf{A} = \mathbf{I}$ on $P(t)$,

$$\mathbf{u}|_{t=0} = \mathbf{u}_{0,h} \quad \text{in } \Omega,$$

$$\mathbf{A}_h|_{t=0} = \mathbf{A}_{0,h} \quad \text{in } \Omega. \quad (32)$$

In our numerical scheme, since the motion inside the particles is rigid body like, the value of configuration tensor inside the particles is explicitly constrained to be equal to \mathbf{I} .

4. Time discretization using the Marchuk-Yanenko operator splitting scheme

The initial value problem (32) is solved by using the Marchuk-Yanenko operator splitting scheme which allows us to decouple its four primary difficulties:

1. The incompressibility condition, and the related unknown pressure p_h ,
2. The nonlinear advection term,
3. The constraint of rigid-body motion in $P_h(t)$, and the related distributed Lagrange multiplier $\boldsymbol{\lambda}_h$,
4. The equation for the configuration tensor, and the viscoelastic stress tensor which appears in the momentum equation.

The Marchuk-Yanenko operator splitting scheme can be applied to an initial value problem of the form

$$\frac{d\phi}{dt} + A_1(\phi) + A_2(\phi) + A_3(\phi) + A_4(\phi) = f$$

where the operators $A_1, A_2, A_3,$ and A_4 can be multiple-valued. Let Δt be the time step, and α, β and γ be three constants: $0 \leq \alpha, \beta, \gamma \leq 1$ and $\alpha + \beta + \gamma = 1$. We use the following version of the Marchuk-Yanenko operator splitting to simulate the motion of particles in a viscoelastic fluid:

Set $\mathbf{u}^0 = \mathbf{u}_{0,h}, \mathbf{A}^0 = \mathbf{A}_{0,h}, \mathbf{U}^0 = \mathbf{U}_0, \mathbf{X}^0 = \mathbf{X}_0$ and $\omega^0 = \omega_0$.

For $n=0,1,2,\dots$ assuming $\mathbf{u}^n, \mathbf{A}^n, \mathbf{U}^n, \mathbf{X}^n,$ and ω^n are known, find the values for $n+1$ using the following:

STEP 1:

Find $\mathbf{u}^{n+1/4} \in W_{\Gamma,h}^{n+1}$ and $p^{n+1/4} \in L_{0,h}^2$, by solving

$$\begin{aligned} \int_{\Omega} \rho_L \frac{\mathbf{u}^{n+1/4} - \mathbf{u}^n}{\Delta t} \cdot \mathbf{v} \, dx - \int_{\Omega} p^{n+1/4} \nabla \cdot \mathbf{v} \, dx + \alpha \int_{\Omega} 2\eta_s \mathbf{D}[\mathbf{u}^{n+1/4}] : \mathbf{D}[\mathbf{v}] \, dx &= \int_{\Omega} \mathbf{v} \cdot \nabla \cdot \left(\frac{\mathbf{c}}{\lambda_s} \mathbf{A}^n \right) \, dx \\ &\text{for all } \mathbf{v} \in W_{0,h}, \\ \int_{\Omega} q \nabla \cdot \mathbf{u}^{n+1/4} \, dx &= 0 \quad \text{for all } q \in L_h^2, \end{aligned} \quad (33)$$

STEP 2:

Find $\mathbf{u}^{n+2/4} \in W_{\Gamma,h}^{n+1}$, by solving

$$\begin{aligned} \int_{\Omega} \rho_L \frac{\mathbf{u}^{n+2/4} - \mathbf{u}^{n+1/4}}{\Delta t} \cdot \mathbf{v} \, dx + \int_{\Omega} \rho_L (\mathbf{u}^{n+2/4} \cdot \nabla \mathbf{u}^{n+2/4}) \cdot \mathbf{v} \, dx + \beta \int_{\Omega} 2\eta_s \mathbf{D}[\mathbf{u}^{n+2/4}] : \mathbf{D}[\mathbf{v}] \, dx &= 0 \\ &\text{for all } \mathbf{v} \in W_{0,h} \end{aligned} \quad (34)$$

STEP 3:

Find $\mathbf{A}^{n+3/4} \in W_{A,h}^{n+1}$, by solving

$$\begin{aligned} \int_{\Omega} \left(\frac{\mathbf{A}^{n+3/4} - \mathbf{A}^n}{\Delta t} + \mathbf{u}^{n+2/4} \cdot \nabla \mathbf{A}^{n+3/4} - \mathbf{A}^{n+3/4} \cdot \nabla \mathbf{u}^{n+2/4} - (\nabla \mathbf{u}^{n+2/4})^T \cdot \mathbf{A}^{n+3/4} + \frac{1}{\lambda_r} (\mathbf{A}^{n+3/4} - \mathbf{I}) \right) \cdot \mathbf{s} \, dx &= 0 \\ &\text{for all } \mathbf{s} \in W_{A0,h}^{n+1} \text{ and } \mathbf{A} = \mathbf{I} \text{ on } P_h(t). \end{aligned} \quad (35)$$

STEP 4:

Compute $\mathbf{U}^{n+2/4}$ and $\mathbf{X}^{n+2/4}$ using the prediction procedure

Set $\mathbf{U}^{n,0} = \mathbf{U}^n, \mathbf{X}^{n,0} = \mathbf{X}^n$.

Do $k=1, K$

$$\mathbf{U}^{*n,k} = \mathbf{U}^{n,k-1} + \left(\mathbf{g} + \left(1 - \frac{\rho_L}{\rho_d} \right)^{-1} \mathbf{M}^{-1} \mathbf{F}'(\mathbf{X}^{n,k-1}) \right) \frac{\Delta t}{K}$$

$$\begin{aligned}\mathbf{X}^{*n,k} &= \mathbf{X}^{n,k-1} + \left(\frac{\mathbf{U}^{n,k-1} + \mathbf{U}^{*n,k}}{2} \right) \frac{\Delta t}{K} \\ \mathbf{U}^{n,k} &= \mathbf{U}^{n,k-1} + \left(\mathbf{g} + \left(1 - \frac{\rho_L}{\rho_d} \right)^{-1} \mathbf{M}^{-1} \frac{\mathbf{F}'(\mathbf{X}^{n,k-1}) + \mathbf{F}'(\mathbf{X}^{*n,k-1})}{2} \right) \frac{\Delta t}{K} \\ \mathbf{X}^{n,k} &= \mathbf{X}^{n,k-1} + \left(\frac{\mathbf{U}^{n,k-1} + \mathbf{U}^{n,k}}{2} \right) \frac{\Delta t}{K}\end{aligned}$$

end do

$$\text{Set } \mathbf{U}^{n+2/4} = \mathbf{U}^{n,K}, \mathbf{X}^{n+2/4} = \mathbf{X}^{n,K}. \quad (36)$$

Find $\mathbf{u}^{n+1} \in W_{u\Gamma,h}^{n+1}$, $\boldsymbol{\lambda}^{n+1} \in \Lambda_h((n+2/4)\Delta t)$, $\mathbf{U}^{n+1} \in \mathbf{R}^2$, and $\boldsymbol{\omega}^{n+1} \in \mathbf{R}$, satisfying

$$\begin{aligned} \int_{\Omega} \rho_L \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+2/4}}{\Delta t} \cdot \mathbf{v} \, dx + \left(1 - \frac{\rho_L}{\rho_d} \right) \left(\mathbf{M} \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n+2/4}}{\Delta t} \cdot \mathbf{V} + \mathbf{I} \frac{\boldsymbol{\omega}^{n+1} - \boldsymbol{\omega}^{n+2/4}}{\Delta t} \cdot \boldsymbol{\xi} \right) + \\ \gamma \int_{\Omega} 2\eta_s \mathbf{D}[\mathbf{u}^{n+1}] : \mathbf{D}[\mathbf{v}] \, dx = \left\langle \boldsymbol{\lambda}^{n+1}, \mathbf{v} - (\mathbf{V} + \boldsymbol{\xi} \times \mathbf{r}^{n+2/4}) \right\rangle_{P((n+2/4)\Delta t)} \end{aligned}$$

for all $\mathbf{v} \in W_{0,h}$, $\mathbf{V} \in \mathbf{R}^2$, and $\boldsymbol{\xi} \in \mathbf{R}$

$$\left\langle \boldsymbol{\mu}_h, \mathbf{u}^{n+1} - (\mathbf{U}^{n+1} + \boldsymbol{\omega}^{n+1} \times \mathbf{r}) \right\rangle_{P((n+2/4)\Delta t)} = 0 \quad \text{for all } \boldsymbol{\mu}_h \in \Lambda((n+2/4)\Delta t), \quad (37)$$

where the center of particle $P((n+2/4)\Delta t)$ is at $\mathbf{X}^{n+2/4}$.

Set $\mathbf{X}^{n+1,0} = \mathbf{X}^n$.

Do $k=1,K$

$$\begin{aligned}\mathbf{X}^{*n+1,k} &= \mathbf{X}^{n+1,k-1} + \left(\frac{\mathbf{U}^n + \mathbf{U}^{n+1}}{2} \right) \frac{\Delta t}{K} \\ \mathbf{X}^{n,k} &= \mathbf{X}^{*n,k-1} + \left(1 - \frac{\rho_L}{\rho_d} \right)^{-1} \mathbf{M}^{-1} \left(\frac{\mathbf{F}'(\mathbf{X}^{n+1,k-1}) + \mathbf{F}'(\mathbf{X}^{*n+1,k})}{2} \right) \frac{(\Delta t)^2}{2K}\end{aligned}$$

end do

$$\text{Set } \mathbf{X}^{n+1} = \mathbf{X}^{n+1,K}. \quad (38)$$

Set $\mathbf{A}^{n+1} = \mathbf{A}^{n+3/4}$, $p^{n+1} = p^{n+1/4}$, and go back to the first step.

Remarks:

1. The first step gives rise to a Stokes-like problem for the velocity and pressure distributions which is solved by using a conjugate gradient method [9].

2. The second step is a nonlinear problem for the velocity which is solved by using a least square conjugate gradient algorithm [9].
3. The third step is a linearized hyperbolic problem for the configuration tensor or stress. This problem is solved by using a third order upwinded positive only scheme [10-14]. The two key features of this scheme are: a positive only scheme that guarantees the positive definiteness of the configuration tensor, and a third order upwinding scheme for discretizing the convection term in the constitutive equation. These two features are important for obtaining a scheme that is stable at relatively large Deborah numbers.
4. The fourth step is used to obtain the distributed Lagrange multiplier that enforces rigid body motion inside the particles. This problem is solved by using a conjugate gradient method described in [1,7]. In our implementation of the method we have used an H^1 inner product (see (24)) for obtaining the distributions over the particles, as the discretized velocity is in H^1 .

5. Results

We next discuss the numerical results obtained using the above algorithm for the motion of rigid particles suspended in the Oldroyd-B fluid. In our implementation of scheme (33-38), $\alpha = \beta = 0.5$ and $\gamma=0$. The parameter c in the Oldroyd-B model will be assumed to be one, i.e., $\eta_s = \eta_p$. The parameter ρ in the particle-particle and particle-wall force models is equal to one and half times the velocity mesh size. We will also assume that all dimensional quantities are in the CGS units.

5.1 Sedimentation of a single particle

We begin by investigating the case of a single circular particle sedimenting in a channel filled with the Oldroyd-B fluid. The objective of this study is to show that results are independent of the mesh resolution and the time step. We will assume that $\lambda_r = 0.01$, $\eta = 0.01$ and $\rho_L = 1.0$, and the particle diameter and density are 0.2 and 1.5, respectively. The initial state of the stress and velocity in the fluid, and the particle velocity are:

$$\begin{aligned}
\mathbf{u}_0 &= \mathbf{0}, \\
\mathbf{A}_0 &= \mathbf{I}, \\
\mathbf{U}_{i0} &= \mathbf{0}, \\
\boldsymbol{\omega}_{i0} &= \mathbf{0}.
\end{aligned} \tag{39}$$

The initial value $\mathbf{A}_0 = \mathbf{I}$ implies that the Oldroyd-B fluid is in a relaxed state. The channel width is 1.5 and height is 6. The simulations are started at $t=0$ by dropping a single particle at a distance of 0.375 from the center of the channel and at a height of 5.2.

We have used two regular triangular meshes to show that the results converge with mesh refinement. In a triangular element there are six velocity and three pressure nodes. Therefore, the size

of the velocity elements is one half of that of the pressure elements. The particle domain is also discretized using a triangular mesh similar to the one used in [6]. The size of the velocity elements for the first mesh is $1/96$, and for the second mesh is $1/128$. The size of the particle elements for the first mesh is $1/70$, and for the second mesh is $1/120$. The number of velocity nodes and elements in the first mesh are 83665 and 41472, respectively. In the second mesh, there are 148417 velocity nodes and 73728 elements. The time step for these simulations is fixed, and assumed to be 0.001 or 0.0004.

In figure 3 we have shown the x and y-components of velocity and angular velocity as a function of time. These results are obtained for the two meshes described above using the time steps of 0.001 and 0.0004. From this figure we note that the particle accelerates downwards until it reaches its maximum fall velocity at $t \approx 0.25$, called the terminal velocity. After reaching the terminal velocity, the particle falls with an approximately constant velocity. The Reynolds number for the particle is around 180 and $De=0.45$. The particle also rotates in the clockwise direction. The angular velocity of the particle also fluctuates slightly with time, especially for $t > 0.1$ because of the wake bubble behind the particle is unstable. These fluctuations imply that the problem is not completely steady even in the frame attached to the particle. It is noteworthy that since the linear and angular velocities of a falling cylinder are functions of time, these results cannot be compared with the well-known results for the flow past a fixed cylinder. The accuracy of the DLM method for the case of a single particle immersed in a steady Stokes fluid in two dimensions and with a known rigid-body motion has been analyzed in [15]. It was shown that the order of error of velocity field is about $1/2$ less than that for a boundary fitted mesh due to the loss of regularity of solution which is extended in the fictitious domain. This loss of accuracy can be easily compensated by using a finer mesh. Also note that it is worth to pay this price for the simplification in the implementation of the DLM method, especially in the parallelization of three-dimensional codes.

From figure 3 we note that when the number of nodes used is approximately doubled the y-component of velocity remains approximately the same (see curves marked ++ and +++). The x-component of velocity u and the angular velocity ω , on the other hand, are approximately equal only for $t < 0.1$. The motion of particle for $t > 0.1$ is influenced by the unstable wake bubble, especially the side ways motion and the angular velocity, and thus the results are sensitive to the mesh size and the time step. Therefore, we may conclude that for $t < 0.1$ —the time duration for which the wake bubble does not influences the motion of particle—the results are independent of the mesh resolution. Similarly, a comparison of the curves marked (+) and (+++) shows that when the time step is reduced by a factor of 2.5 the temporal evolutions of the particle velocity, angular velocity, and trajectory do not change significantly which shows that the results are also independent of the time step for $t < 0.1$.

The y-component of velocity can be used to obtain the drag coefficient for the particle after it reaches the terminal velocity. Since the Reynolds number is around 180, the drag coefficient must be of $O(1)$. For the above case the drag coefficient is approximately 1.9, where the drag coefficient is defined to be

$$C_d = \frac{\frac{1}{4} \pi D^2 (\rho_p - \rho_L) g}{\frac{1}{2} \rho_L U^2 D}.$$

In figures 4-6 the velocity and $\text{tr}\mathbf{A}$ distributions are shown at $t \approx 0.3$, i.e., after the particle reaches its terminal velocity. The trace of configuration tensor is used to show the distribution of normal stresses; In the state of equilibrium $\text{tr}\mathbf{A}$ is 2 (in two-dimensions). Also note that since all flows become viscometric at a solid wall, on the boundary of a solid particle the extra stress is zero and $\text{tr}\mathbf{A}$ is equal to $2 + 2 (\dot{\gamma} \lambda_r)^2$, where $\dot{\gamma}$ is the shear rate. This feature has been used in [16] to explain forces that produce stable chains. From figures 4b, 5b and 5c we note that $\text{tr}\mathbf{A}$ is large in front of the particle, and also behind the particle in the region outside the wake bubble. Inside the wake bubble since the rate of extension is small, $\text{tr}\mathbf{A}$ is also small. From figures 4 and 5, where the results for two different mesh resolutions are shown, we note that the qualitative features of the velocity and $\text{tr}\mathbf{A}$ distributions are the same. Similarly, from figures 4 and 6, where the results obtained for the same mesh using two different time steps of 0.001 and 0.0004 are shown, we note that the distributions are qualitatively similar. The velocity and $\text{tr}\mathbf{A}$ distributions, however, as noted before, are not identical because of the unstable wake bubble.

In order to investigate the role of wake bubble on the qualitative nature of $\text{tr}\mathbf{A}$ distribution, we studied the sedimentation of a particle with $\rho_p = 1.02$ and $\lambda_r = 0.3$. The remaining parameters are the same as above. The terminal velocity of the particle in this case is approximately 1.59. Note that the terminal velocity in this case is much smaller because the particle density is only 2% larger than the fluid density. The Reynolds number for the particle is around 31.8 and $De = 2.4$. From the velocity distribution shown in figure 7a we note that since the Reynolds number is not too large, the size of the wake bubble is considerably smaller. Thus, the qualitative features of the $\text{tr}\mathbf{A}$ distribution in figure 7b are significantly different from that of figures 4-6. Also note that the regions of large values of $\text{tr}\mathbf{A}$ on the two sides of particle merge together behind the particle, indicating that the wake bubble size is small compared to the length scale associated with the viscoelastic flow. The hyperbolic nature of the constitutive equation for the stress implies that the viscoelastic fluid around the particle takes a time of $O(\lambda_r)$ to relax back to the state of equilibrium. Since for our simulation De is 2.4, the time taken by the fluid to relax back to the state of equilibrium is longer than the time scale associated with the particle

motion. Therefore, there is a region behind the particle in which the viscoelastic stresses are relatively large. This slow relaxation of the fluid influences the motion of trailing particles.

5.2 Sedimentation of two cylindrical particles in a channel

It is well known that when two particles are dropped close to each other in a Newtonian fluid they interact undergoing repeated drafting, kissing and tumbling [17,18]. This problem can be investigated using our code by assuming that $\lambda_r = 0$. For these simulations the channel width is 2 and height is 8. The velocity elements size is 1/96, and the size of the particle elements is 1/70. We will assume that $\eta = 0.01$ and $\rho_L = 1.0$, and the particle diameter and density are 0.2 and 1.01, respectively. The simulations are started at $t=0$ by dropping two particles at the center of the channel at $y= 7.2$ and 6.8. From figure 8a we note that the particle on the top drafts in the wake of the lower particle. The particles fall with an average velocity of 1.4. The Reynolds number for the particles in this case is 24. Since the drag acting on the particle in the wake is smaller, it falls more rapidly than the particle in front. This causes them to touch or kiss (see figure 8b). The tumbling of particles takes place because the configuration where they are aligned parallel to the flow direction is unstable (see figure 8c).

When the particles sediment in a viscoelastic liquid, on the other hand, the stable configuration is the one where the particles are aligned parallel to the flow direction. Thus, the particles form chains in the direction parallel to the flow. In Figures 9a and b, the positions of the two particles, and the velocity and $\text{tr}\mathbf{A}$ distributions, are shown at $t=0.5$. They were dropped at a distance of $2D$ from each other at $t=0$. The fluid density is 1.0, and the particle density is 1.01. The fluid viscosity is 0.12 and relaxation time is 1.4, and the particle diameter is 0.2. The $\text{tr}\mathbf{A}$ distribution after the particles have reached an approximately constant terminal velocity of 0.135 is shown in figure 9c. The Reynolds number for the particle is 0.23 and the $De=0.975$. Also note that since the velocity of particle on the top is larger, the distance between them decreases with time. The distance decreases to approximately $D/2$ at $t=9.5$. From Figure 9c, where we have shown the isovalues of $\text{tr}\mathbf{A}$, we note that $\text{tr}\mathbf{A}$ in front of the leading particle and around the particles is relatively large. This figures also shows that it takes some time for the fluid to relax back to the state of equilibrium. This gives rise to the characteristic streak lines (see figures 9b and c) that are indicative of the hyperbolic nature of the constitutive equation for the stress. The particles continue to move closer to each other, and are at a distance of $D/8$ from each other at $t=25$ (see figure 9d).

For the above case since the Deborah number is 0.975 and the average Reynolds number is 0.23, the Mach number is 0.43 and the elasticity number is 4.55. Therefore, there is a strong tendency for the particles to align parallel to the falling direction. But, since the channel length is not very large, the distance between the two particles is decreasing even at $t=25$ and a steady state distance is not reached.

5.3 Sedimentation of eleven cylindrical particles in a channel

Next, we consider the sedimentation of eleven particles in a channel with width 2 and height 8. The fluid density is 1.0, and the particle density is 1.01. The fluid viscosity is 0.13 and relaxation time is 1.3, and the particle diameter is 0.2. The velocity element size is $1/96$, and the size of the particle elements is $1/70$. The simulations are started at $t=0$ by placing the particles in a periodic arrangement at the center of the channel at an average height of 6.8. The particles are dropped with zero linear and angular velocities, and the fluid is in the quiescent relaxed state. The average sedimentation velocity of particles in this case is 0.2. This implies that the average Deborah number is 1.3, and the average Reynolds number is 0.31. Therefore, the Mach number is 0.63 and the elasticity number is 4.19. The distribution of $\text{tr}\mathbf{A}$ and the particle positions at $t=1$ and 15.6 are shown in figure 10a and b, respectively. We note that the particles can be divided into two groups of chains that are approximately parallel to the y -direction, i.e. the direction of fall. The magnitude of $\text{tr}\mathbf{A}$ is relatively large around the two chains, which is similar to the case for two particles.

The simulations were also carried out for the case where the relaxation time is 3.5, the viscosity is 0.3, and the particle density is 1.02. The velocity element size is $1/144$ and the particle mesh size is $1/120$. The remaining parameters are the same as above. The simulations were started with the same initial conditions as above. The average sedimentation velocity of particles in this case is 0.25, and thus the average Deborah number is 4.4, and the average Reynolds number is 0.17. The Mach number is 0.73 and the elasticity number is 26.25. The distribution of $\text{tr}\mathbf{A}$ and the particle positions at $t=15.6$ are shown in figure 10c. We note that in the middle of this figure there are four particles that are aligned approximately vertically, i.e., parallel to the sedimentation direction. Also, note that compared to the case discussed above the particles of chain are closer to each other. In our simulations, the particles are kept apart by one and half times the velocity element size by the repulsive force (14). Therefore, the closest approach of the particles depends on the mesh resolution. The particle chains in our case are, however, relatively less organized than in [5] where the domain is periodic and the particles were allowed to fall over much larger distances. Also note that in the present implementation of (33-38) the mesh is assumed to be uniform which allows us to use a matrix-free fast solver. The obvious disadvantage of a uniform mesh is that it does not allow for a greater resolution near the surfaces of colliding particles.

The simulations were also carried out in a narrow channel with width 1 and height 8. The fluid density is 1.0, and the particle density is 1.01. The fluid viscosity is 0.1 and relaxation time is 3.0, and the particle diameter is 0.2. The average velocity of fall for the particles in this case is 1.0 (see figure 11). Therefore, the average Deborah number is 15, the average Reynolds number is 2.0, the Mach number is 5.48 and the elasticity number is 1.65. Therefore, we do not expect particles to align parallel

to the direction of fall. But, since in this the channel width is also relatively small, the particles interact with the walls and fall without having any noticeable structure.

5.4 Fluidization of 102 particles

Finally we consider the fluidization of 102 particles in a channel with width 2 and height 8. The fluid density is 1.0, and the particle density is 1.01. The fluid viscosity is 0.02 and relaxation time is 0.5, and the particle diameter is 0.2. The velocity elements size is $1/96$, and the size of the particle elements is $1/70$. The particles are arranged in a periodic arrangement at the bottom of the bed. The simulations are started at $t=0$ by suddenly starting the Poiseuille flow in the channel to fluidize particles. The centerline velocity at the inlet is 0.5. Before the flow is started, the particles have zero linear and angular velocities and the fluid is in the quiescent relaxed state. The particles are fluidized by the incoming flow, as the drag acting on the particles is larger than their buoyant weight. In figure 12 the distribution of particle and trA is shown at $t=2$. From this figure we note that the particles near the walls form chains parallel to the wall. But, away from the walls the relative orientation is relatively less organized, i.e., the distribution of particles appears to be random. The random distribution of particles in the middle of the bed may be a consequence of the complex particle-particle interactions. Close to the walls, we expect these particle-particle interactions to be far less important, and thus the viscoelastic stresses are sufficient to align the particles parallel to the flow direction.

6. Conclusions

The distributed Lagrange multiplier/fictitious domain method developed in this paper can be used to efficiently compute the motion of rigid particles suspended in the Oldroyd-B fluid. The method is implemented using a combined weak formulation where the forces and moments between the particles and fluid cancel, as they are internal to the combined system. The governing equations for the Oldroyd-B liquid are solved everywhere in the domain, including inside the particles, and the rigid body motion inside the particles is enforced using a distributed Lagrange multiplier method. The Marchuk-Yanenko operator-splitting technique is used to decouple the difficulties associated with the incompressibility constraint, and the nonlinear convection and viscoelastic terms. The constitutive equation is solved using a scheme that uses a third order upwind discretization for the convection term and guarantees the positive definiteness of the configuration tensor.

In order to validate our code we have simulated the sedimentation of a single particle. We have verified that the results are independent of the mesh resolution as well as the size of time step. Our simulations show that when two or more particles are dropped in a channel, and the Mach number (Ma) is less than one and the elasticity number (E) is greater than one, the particles chain along the flow direction, which is in agreement with the results presented in [2]. Our simulations of fluidization

of 102 particles in a two dimensional bed show that the particles form chains along the channel walls, and away from the channel walls the orientation of particles is relatively random.

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8. Figures

Figure 1. A typical rectangular domain used in our simulations; Γ^- is the upstream portion of Γ .

Figure 2. The imaginary particle used for computing the repulsive force acting between a particle and a wall.

Figure 3. The velocity components u and v , and the angular velocity ω are shown as a function of time. (+) The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.001 . (++) The size of the velocity elements is $1/144$, and the size of the particle elements is $1/120$. The time step is 0.0004 . (+++) The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.0004 .

Figure 4. The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.001 and $t=0.303$ (a) the velocity field, (b) isovalues of $\text{tr}\mathbf{A}$.

Figure 5. The size of the velocity elements is $1/128$, and the size of the particle elements is $1/120$. The time step is 0.0004 and $t=0.304$ (a) the velocity field, (b) isovalues of $\text{tr}\mathbf{A}$.

Figure 6. The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.0004 and $t=0.327$. (a) the velocity field, (b) isovalues of $\text{tr}\mathbf{A}$.

Figure 7. The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.0004 and $t=3.1$. (a) the velocity field, (b) isovalues of $\text{tr}\mathbf{A}$.

Figure 8. For $De=0$ the velocity field is shown. The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.0004 . The two particles are dropped at $t=0$ at $y=7.7$ and $y=6.6$. The particles undergo the characteristic drafting kissing and tumbling. (a) $t=0.5$ (b) $t=9.5$ and (c) $t=25$.

Figure 9. The size of the velocity elements is $1/96$, and the size of the particle elements is $1/70$. The time step is 0.0004 . The two particles are dropped at $t=0$ at $y=7.7$ and $y=6.6$. (a) The velocity field at $t=0.5$, (b) Isovalues of $\text{tr}\mathbf{A}$ at $t=0.5$, (c) Isovalues of $\text{tr}\mathbf{A}$ at $t=9.5$, (d) Isovalues of $\text{tr}\mathbf{A}$ at $t=25$.

Figure 10. Sedimentation of eleven particles in a wide channel is shown. (a) Isovalues of $\text{tr}\mathbf{A}$ at $t=1$, (b) Isovalues of $\text{tr}\mathbf{A}$ at $t=15.6$. (c) Isovalues of $\text{tr}\mathbf{A}$ at $t=18.3$.

Figure 11. Sedimentation of eleven particles in a narrow channel is shown. Isovalues of $\text{tr}\mathbf{A}$ at $t=21.1$.

Figure 12. Fluidization of 102 particles in a two dimensional bed. Isovalues of trA at $t=2$.