3D DLM/FD METHODS FOR SIMULATING THE MOTION OF SPHERES IN BOUNDED SHEAR FLOWS OF OLDROYD-B FLUIDS

A Dissertation

Presented to

the Faculty of the Department of Mathematics

University of Houston

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

By

Shang-Huan Chiu

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Abstract

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CHAPTER 1

Introduction

Suspensions of particles in fluids appear in many applications of chemical, biological, petroleum, and environmental areas. For the dynamics of rigid non-Brownian particles suspended in viscoelastic fluids, peculiar phenomena of the particle motion and pattern induced by fluid elasticity have been reviewed on theoretical predictions, experimental observations and numerical simulations from the existing papers in [6]

In Newtonian fluid, plenty numerical and experimental results have been published. Several topics are considered, such as the random displacements resulting from particle encounters under creeping-flow conditions and the rotation of a neutrally buoyant particle in simple shear flow. The displacements from particle encounters lead to hydrodynamically induced particle migration, which constitutes an important mechanism for particle redistribution in the suspending fluid (see, e.g., [21] and the references therein). Binary encounters of particles is a phenomenon have been found that two balls either pass each other or swapping their cross streamline position.

But particle suspensions in viscoelastic fluids have different behaviors, e.g., strings of spherical particles aligned in the flow direction (e.g., see [12, 16, 19, 14]) and 2D crystalline patches of particles along the flow direction [15] in shear flow. As mentioned in [17], 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. Furthermore, 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 [16, 19]. There are numerical studies of the two particle interaction and aggregation in viscoelastic fluids(e.g., see [8, 3, 20]). Several non-Newtonian fluid models in bounded shear flow have been considered, such as Oldroyd-B fluid, Giesekus fluid.

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 [20]. We have further tested the cases of two balls for the Weissenberg number up to 1 and obtained they either pass, return, or tumble in a bounded shear flow with two moving wall. The trajectories of the two ball mass centers lose the symmetry due to the effect of elastic force arising from viscoelastic fluids for the higher values of the Weissenberg number. For the interaction of the two balls in one wall driven shear flow, two balls form a loosely connected chain if the initial gap between two balls is small enough and then these two balls keep rotating with respect to the midpoint between their mass centers and migrate toward the moving wall.

DLM/FD Method

To simulate the interaction of neutrally buoyant balls in 3D bounded shear flow of Oldroyd-B fluids, we have generalized a distributed Lagrange multiplier/fictitious domain method (DLM/FD) developed in [13] for simulating the motion of neutrally buoyant particles in Stokes flows of Newtonian fluids from 2D to 3D and then combined such method with the operator splitting scheme and matrix-factorization approach for treating numerically the constitutive equations of the conformation tensor of Oldroyd-B fluids. In this matrix-factorization approach, which is the technique close to the one developed by Lozinski and Owens in [11],

CHAPTER 2

3D DLM/FD methods for simulating the motion of spheres in bounded shear flows of Newtonian fluids

2.1 Stokes Equations and Newtonian Model

Consider the Stokes equations in $\Omega \times (0, T)$ describing the 3-dimensional motion of an incompressible and isothermal fluid without body force:

$$\begin{cases} -\nabla \cdot \sigma = \rho_f \mathbf{g}, \\ \nabla \cdot \mathbf{u} = 0. \end{cases}$$

where $\sigma = -p\mathbf{I} + \boldsymbol{\tau}$ with presure p and stress tensor $\boldsymbol{\tau}$, $\mathbf{u} = (u_1, u_2, u_3)$ is the flow velocity, $\mathbf{g}$ is the gravity, and ρ_f is the density of fluid.

The constitutive equation of the stress tensor is given by

$$\tau = 2\mu\mathbf{D}(\mathbf{u})$$

where μ is the Newtonian viscosity of the fluid and $\mathbf{D}(\mathbf{u})$ is the symmetric rate of strain tensor

$$\mathbf{D}(\mathbf{u}) = \frac{\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathbf{T}}}{\mathbf{2}},$$

with the Jacobian of the velocity $\nabla\mathbf{u}$,

$$\nabla\mathbf{u} = \begin{bmatrix} \frac{\partial u_1}{\partial x} & \frac{\partial u_1}{\partial y} & \frac{\partial u_1}{\partial z} \\ \frac{\partial u_2}{\partial x} & \frac{\partial u_2}{\partial y} & \frac{\partial u_2}{\partial z} \\ \frac{\partial u_3}{\partial x} & \frac{\partial u_3}{\partial y} & \frac{\partial u_3}{\partial z} \end{bmatrix}$$

2.2 DLM/FD Method for Simulating Fluid-particle Interaction in Stokes Flow

2.2.1 The Governing Equations

Let Ω be a bounded domain in $\mathbb{R}^3$ and let Γ be the boundary of Ω. We suppose that Ω is filled with a viscous fluid with density ρ_f and contains N moving particles of density ρ_s. Let $B(t) = \bigcup_{i=1}^{N} B_i(t)$ where $B_i(t)$ is the i-th soild particle in the fluid for

$i = 1, 2, \cdots, N$. We denote by $\gamma_i(t)$ the boundary $\partial B_i(t)$ of $B_i(t)$ for $i = 1, 2, \cdots, N$ and let $\gamma(t) = \bigcup_{i=1}^{N} \gamma_i(t)$.

For some $T > 0$, the governing equations for the fluid-particles system is as follows:

For the motion of fluid, we consider the Stokes equations in Oldroyd-B model:

$$-\nabla \cdot \sigma = \rho_f \mathbf{g} \quad \text{in } \Omega \setminus \overline{B(t)}, t \in (0, T), \tag{2.2.1}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \setminus \overline{B(t)}, t \in (0, T), \tag{2.2.2}$$

$$\mathbf{u} = \mathbf{g_0} \quad \text{on } \Gamma \times (0, T), \text{with } \int_\Gamma \mathbf{g_0} \cdot \mathbf{n} d\Gamma = 0, \tag{2.2.3}$$

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{V}_i(t) + \omega_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \mathbf{x} \in \gamma_i(t),\, i = 1, 2, \cdots, N, \tag{2.2.4}$$

where $\mathbf{u}$ is the flow velocity, p is the presure, $\mathbf{g}$ is the gravity, $\sigma = -p\mathbf{I} + \tau_s$, $\tau_s = 2\mu_f \mathbf{D}(\mathbf{u})$ is a Newtonian stress tensor, ρ_f is the density of fluid and μ_f is the solvent viscosity of the fluid, and $\mathbf{n}$ is the unit normal vector pointing outward to the flow region.

In (2.2.4), we assume a no-slip condition on $\gamma(t)$:

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{V}_i(t) + \omega_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \mathbf{x} \in \gamma_i(t),\, i = 1, 2, \cdots, N,$$

where $\mathbf{V}_i$ is the translation velocity, ω_i is the angular velocity, $\mathbf{G_i}$ is the center of mass and $\mathbf{x}$ is a point on the surface of the particle.

In (2.2.1), we use $\sigma = -p\mathbf{I} + 2\mu_f \mathbf{D}(\mathbf{u})$ and obtain

$$\nabla p - 2\mu_f \nabla \cdot \mathbf{D}(\mathbf{u}) = \rho_f \mathbf{g}. \tag{2.2.5}$$

The motion of particle satisfies the Euler-Newton's equations:

$$\mathbf{v}_i(\mathbf{x}, t) = \mathbf{V}_i(t) + \boldsymbol{\omega}_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \{\mathbf{x}, t\} \in \overline{B_i(t)} \times (0, T),\ i = 1, 2, \cdots, N, \tag{2.2.6}$$

$$\frac{\mathrm{d}\mathbf{G}_i}{\mathrm{d}t} = \mathbf{V}_i, \tag{2.2.7}$$

$$M_i \frac{\mathrm{d}\mathbf{V_i}}{\mathrm{d}t} = M_i \mathbf{g} + \mathbf{F}_i + \mathbf{F}_i^r, \tag{2.2.8}$$

$$\frac{\mathrm{d}(\mathbf{I_i}\boldsymbol{\omega}_\mathbf{i})}{\mathrm{d}t} = \mathbf{T}_i + \overrightarrow{\mathbf{G}_i\mathbf{x}_r} \times \mathbf{F}_i^r, \tag{2.2.9}$$

$$\mathbf{G}_i(0) = \mathbf{G}_i^0,\ \mathbf{V}_i(0) = \mathbf{V}_i^0,\ \omega_i(0) = \omega_i^0, \tag{2.2.10}$$

for $i = 1, 2, \cdots, N$, where M_i and I_i are the mass and the moment of inertia of the i-th particle, respectively; $\mathbf{F}_i$ and $\mathbf{T}_i$ are the hydrodynamical force and torque imposed on the i-th particle by the fluid, and $\mathbf{F}_i^r$ is a short range repulsion force imposed on the i-th particle by other particles and wall to prevent particle/particle and particle/wall penetration.

The hydrodynamical force $\mathbf{F}_i$ and torque $\mathbf{T}_i$ imposed on the i-th particle by the fluid are given by

$$\mathbf{F}_i = -\int_\gamma \sigma \mathbf{n}\, \mathrm{d}\gamma, \quad \mathbf{T}_i = -\int_\gamma \overrightarrow{\mathbf{G}_i\mathbf{x}} \times \sigma \mathbf{n}\, \mathrm{d}\gamma.$$

$\overrightarrow{\mathbf{G}_i\mathbf{x}_r} \times \mathbf{F}_i^r$ is a torque acting on the point $\mathbf{x}_r$ where $\mathbf{F}_i^r$ applies on the i-th particle.

2.3 Variational Formulation

For convenience of derivation, we assume there is only one particle in the fluid, that is, we set $B(t)$ the soild particle in the fluid, $\gamma(t)$ the boundary $\partial B(t)$ of $B(t)$, $\mathbf{G}(t)$ the center of mass of this particle. In the equations of the motion of particle, we set $\mathbf{V}$ the translation velocity of the particle $B(t)$, $\boldsymbol{\omega}$ the angular velocity of the particle $B(t)$, M_p and $\mathbf{I_p}$ the mass and the moment of inertia of the particle $B(t)$, respectively; $\mathbf{F}$ and $\mathbf{T}$ the hydrodynamical force and torque imposed on the particle $B(t)$ by the fluid, respectively, and $\mathbf{F}^r$ a short range repulsion force imposed on the particle $B(t)$.

To obtain a variational formulation for above problem (2.2.5),(2.2.2) – (2.2.4), we define the following function spaces

$$\mathbf{W}_{\mathbf{g}_0}(t) = \left\{ \mathbf{v} \,\middle|\, \mathbf{v} \in (H^1(\Omega \setminus \overline{B(t)}))^3, \mathbf{v} = \mathbf{g}_0(t) \,\text{on}\, \Gamma, \mathbf{v} = \mathbf{V}(t) + \omega(t) \times \overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \text{on } \partial B(t) \right\},$$

$$\mathbf{W}_0(t) = \left\{ (\mathbf{v}, \mathbf{Y}, \theta) \,\middle|\, \mathbf{v} \in (H^1(\Omega \setminus \overline{B(t)}))^3, \mathbf{v} = 0 \,\text{on}\, \Gamma, \mathbf{v} = \mathbf{Y} + \theta \times \overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \text{on } \partial B(t), \ \text{with } \ \mathbf{Y} \in \mathbb{R}$$

and

$$L_0^2(\Omega \setminus \overline{B(t)}) = \left\{ q \,\middle|\, q \in L^2(\Omega \setminus \overline{B(t)}), \int_{\Omega \setminus \overline{B(t)}} q \, \mathrm{d}\mathbf{x} = 0 \right\}.$$

Applying the virtual power principle to the system (2.2.5),(2.2.2) – (2.2.4) obtains the following variational formulation:

For a.e. $t > 0$, find $\mathbf{u}(t) \in \mathbf{W}_{\mathbf{g}_0}(t)$, $p(t) \in L_0^2(\Omega \setminus \overline{B(t)})$,$\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\omega(t) \in \mathbb{R}^3$, such that

$$\begin{cases} -\displaystyle\int_{\Omega\setminus\overline{B(t)}} p\nabla\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + 2\mu_f \int_{\Omega\setminus\overline{B(t)}} \mathbf{D}(\mathbf{u}):\mathbf{D}(\mathbf{v})\,\mathrm{d}\mathbf{x} \\ +\left(M_p\dfrac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} - M_p\mathbf{g} - \mathbf{F}^r\right)\cdot\mathbf{Y} \quad + \left(\mathbf{I_p}\dfrac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}t} - \overrightarrow{\mathbf{G}\mathbf{x}_r}\times\mathbf{F}^r\right)\cdot\boldsymbol{\theta} \\ \quad = \rho_f \displaystyle\int_{\Omega\setminus\overline{B(t)}} \mathbf{g}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x}, \quad \forall(\mathbf{v},\mathbf{Y},\boldsymbol{\theta})\in\mathbf{W}_0(t), \end{cases} \tag{2.3.11}$$

$$\int_{\Omega\setminus\overline{B(t)}} q\nabla\cdot\mathbf{u}\,\mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2(\Omega\setminus\overline{B(t)}), \tag{2.3.12}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{2.3.13}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega\setminus\overline{B(0)}, \tag{2.3.14}$$

$$\mathbf{G}(\mathbf{x},0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x},0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x},0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{2.3.15}$$

To obtain an equivalent fictitious domain formulation, first we fill the particle $B(t)$ with a fluid of density ρ_f and suppose that this fluid follows the same rigid body motion as $B(t)$ itself, which is

$$\mathbf{u}(\mathbf{x},t) = \mathbf{V}(t) + \boldsymbol{\omega}(t)\times\overrightarrow{\mathbf{G}(t)\mathbf{x}}, \quad \forall\mathbf{x}\in B(t). \tag{2.3.16}$$

Define a function space

$$\widetilde{\mathbf{W}}_0(t) = \left\{(\mathbf{v},\mathbf{Y},\boldsymbol{\theta})\,\middle|\,(\mathbf{v}|_{\Omega\setminus\overline{B(t)}},\mathbf{Y},\boldsymbol{\theta})\in\mathbf{W}_0(t), \mathbf{v}(\mathbf{x},t) = \mathbf{Y}+\boldsymbol{\theta}\times\overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \forall\mathbf{x}\in B(t)\right\}.$$

Suppose particle B is made of an homogeneous material of density ρ_f which follows

$$\rho_f \int_{B(t)} \mathbf{g} \cdot \mathbf{v} \,\mathrm{d}\mathbf{x} = \frac{\rho_f}{\rho_s} M_p \mathbf{g} \cdot \mathbf{Y}, \quad \forall (\mathbf{v}, \mathbf{Y}, \theta) \in \widetilde{\mathbf{W}}_0(t), \tag{2.3.17}$$

$$\nabla \cdot \mathbf{v} = 0 \text{ in } B(t), \quad \forall (\mathbf{v}, \mathbf{Y}, \theta) \in \widetilde{\mathbf{W}}_0(t), \tag{2.3.18}$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } B(t) \text{ and } \mathbf{D}(\mathbf{u}) = 0 \text{ in } B(t). \tag{2.3.19}$$

To obtain a fictitious domain formulation, we define the following function spaces

$$\mathbf{V}_{\mathbf{g}_0}(t) = \left\{ \mathbf{v} \,\middle|\, \mathbf{v} \in (H^1(\Omega))^3, \mathbf{v} = \mathbf{g}_0(t) \text{ on } \Gamma \right\},$$

$$L_0^2(\Omega) = \left\{ q \,\middle|\, q \in L^2(\Omega), \int_\Omega q \,\mathrm{d}\mathbf{x} = 0 \right\}.$$

Combining (2.3.11)-(2.3.15) with (2.3.16)-(2.3.19), we obtain the fictitious domain formulation as follows:

For a.e. $t > 0$, find find $\mathbf{u}(t) \in \mathbf{V}_{\mathbf{g}_0}(t)$, $p(t) \in L_0^2(\Omega)$, $\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, such that

$$\begin{cases} -\displaystyle\int_\Omega p \nabla \cdot \mathbf{v} \,\mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v}) \,\mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} \cdot \mathbf{Y} + \mathbf{I}_p \dfrac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}t} \cdot \boldsymbol{\theta} - \mathbf{F}^r \cdot \mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r} \times \mathbf{F}^r \cdot \boldsymbol{\theta} \\ = \rho_f \displaystyle\int_\Omega \mathbf{g} \cdot \mathbf{v} \,\mathrm{d}\mathbf{x} + \left(1 - \frac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y}, \\ \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \widetilde{\mathbf{W}}_0(t), \end{cases} \tag{2.3.20}$$

$$\int_\Omega q \nabla \cdot \mathbf{u} \,\mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2(\Omega), \tag{2.3.21}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{2.3.22}$$

$$\mathbf{u}(\mathbf{x},t) = \mathbf{V}(t) + \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G}(t)\mathbf{x}}, \quad \forall \mathbf{x} \in B(t). \tag{2.3.23}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \overline{B(0)}, \tag{2.3.24}$$

$$\mathbf{G}(\mathbf{x},0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x},0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x},0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{2.3.25}$$

To relax the rigid body motion condition (**??**), we introduce a Lagrange multiplier, $\boldsymbol{\lambda} \in \Lambda(t) = (H^1(B(t)))^3$, and for any $\mu \in (H^1(B(t)))^3$ and $\mathbf{v} \in (H^1(\Omega))^3$:

$$\langle \mu, \mathbf{v} \rangle_{\Lambda(t)} = \int_{B(t)} (\mu \cdot \mathbf{v} + \nabla \mu \cdot \nabla \mathbf{v}) \, \mathrm{d}\mathbf{x}.$$

We obtain the fictitious domain formulation with Lagrange multiplier as follows:

For a.e. $t > 0$, find find $\mathbf{u}(t) \in \mathbf{V}_{\mathbf{g}_0}(t)$, $p(t) \in L_0^2(\Omega)$, $\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, $\boldsymbol{\lambda} \in \Lambda(t)$ such that

$$\begin{cases} -\displaystyle\int_\Omega p \nabla \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v}) \, \mathrm{d}\mathbf{x} + M_p \frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} \cdot \mathbf{Y} + \mathbf{I}_p \frac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}t} \cdot \boldsymbol{\theta} \\ \quad -\mathbf{F}^r \cdot \mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r} \times \mathbf{F}^r \cdot \boldsymbol{\theta} - \left\langle \boldsymbol{\lambda}, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}\mathbf{x}} \right\rangle_{\Lambda(t)} \\ \quad = \rho_f \displaystyle\int_\Omega \mathbf{g} \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + \left(1 - \frac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y}, \\ \quad \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in (H_0^1(\Omega))^3 \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{2.3.26}$$

$$\int_\Omega q \nabla \cdot \mathbf{u} \, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2(\Omega), \tag{2.3.27}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{2.3.28}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \overline{B(0)}, \tag{2.3.29}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u}(t) - \mathbf{V}(t) - \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G(t)x}} \right\rangle_{\Lambda(t)} = 0, \, \forall \boldsymbol{\mu} \in \Lambda(t), \tag{2.3.30}$$

$$\mathbf{G}(\mathbf{x},0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x},0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x},0) = \boldsymbol{\omega}_0(\mathbf{x}). \tag{2.3.31}$$

Since $\mathbf{u}$ is divergence free and satisfies the Dirichlet boundary conditions on Γ, we obtain

$$2\int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v}) \, \mathrm{d}\mathbf{x} = \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} \, \mathrm{d}\mathbf{x}, \quad \forall \mathbf{v} \in (H_0^1(\Omega))^3.$$

2.4 Finite Element approximation and Operator Splitting scheme

2.4.1 Finite Element approximation

For the purpose of finding an approximation solution of problem (2.3.26)-(2.3.31), we need a partition of the flow region $\Omega \in \mathbb{R}^3$. We use an uniform finite element mesh for Ω and let h be the uniform finite element mesh size for the velocity field, $\mathcal{T}_h$ be a tetrahedrization of Ω, and $\mathcal{T}_{2h}$ be twice coarser than $\mathcal{T}_h$.

For space discretization, we have chosen P_1-iso-P_2 finite elements for the velocity field and P_1 finite elements for the pressure where P_i is the space of the polynomials in three variables of degree $\leq i$ for $i = 1, 2$.

Then we define the following function spaces:

$$\mathbf{V}_h = \left\{ \mathbf{v}_h \,\middle|\, \mathbf{v}_h \in \left(C^0(\bar{\Omega})\right)^3, \mathbf{v}_h\,|_T \in (P_1)^3, \forall T \in \mathcal{T}_h \right\},$$

$$\mathbf{V}_{\mathbf{g}_{0h}(t)} = \left\{ \mathbf{v}_h \,|\, \mathbf{v}_h \in \mathbf{V}_h, \mathbf{v}_h\,|_\Gamma = \mathbf{g}_{0h}(t) \right\},$$

$$\mathbf{V}_{0h} = \left\{ \mathbf{v}_h \,|\, \mathbf{v}_h \in \mathbf{V}_h, \mathbf{v}_h\,|_\Gamma = 0 \right\},$$

$$L_h^2 = \left\{ q_h \,\middle|\, q_h \in C^0(\bar{\Omega}), q_h\,|_T \in P_1, \forall T \in \mathcal{T}_{2h} \right\},$$

and

$$L_{0h}^2 = \left\{ q_h \,\middle|\, q_h \in L_h^2, \int_\Omega q_h \, \mathrm{d}\mathbf{x} = 0 \right\},$$

where $\mathbf{g}_{0h}(t)$ is an approximation of $\mathbf{g}_h(t)$ satisfying

$$\int_\Gamma \mathbf{g}_{0h}(t) \cdot \mathbf{n} \mathrm{d}\Gamma = 0,$$

and

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

For the space of Lagrange multipier $\Lambda(t)$, we need to define a finite dimensional space to approach $\Lambda(t)$. Let $\{\xi_i\}_{i=1}^N$ be a set of points from $\overline{B(t)}$ which cover $\overline{B(t)}$ evenly. We define the discrete Lagrange multiplier space by

$$\Lambda_h(t) = \left\{ \mu_h \,\middle|\, \mu_h = \sum_{i=1}^N \mu_i \delta(\mathbf{x} - \xi_i), \mu_i \in \mathbb{R}^3, \forall i = 1, \cdots, N \right\},$$

where $\mathbf{x} \to \delta(\mathbf{x} - \xi_i)$ is the Dirac measure at $\mathbf{x} = \xi_i$. For different approaches, there are two different definitions of discretize scalar pairung $< \cdot, \cdot >_{\Lambda_h(t)}$. We will introduce these two scalar pairings in next section.

Baesd on the finite dimensional spaces above, we obtain the following approximation of problem (2.3.26)- (2.3.31) :

For a.e. $t > 0$, find find $\mathbf{u}_h(t) \in \mathbf{V}_{\mathbf{g}_{0h}}(t)$, $p(t) \in L^2_{0h}$, $\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, $\boldsymbol{\lambda}_h \in \Lambda_h(t)$ such that

$$\begin{cases} -\displaystyle\int_\Omega p\nabla \cdot \mathbf{v}\,\mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \nabla \mathbf{u}_h : \nabla \mathbf{v}\,\mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} \cdot \mathbf{Y} + \mathbf{I}_p \dfrac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}t} \cdot \boldsymbol{\theta} - \mathbf{F}^r \cdot \mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r} \times \mathbf{F}^r \cdot \boldsymbol{\theta} \\ = \left(1 - \dfrac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} + \left\langle \boldsymbol{\lambda}_h, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}\mathbf{x}} \right\rangle_{\Lambda_h(t)}, \\ \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{V}_{0h} \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{2.4.32}$$

$$\int_\Omega q\nabla \cdot \mathbf{u}_h\,\mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2_h, \tag{2.4.33}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{2.4.34}$$

$$\mathbf{u}_h(\mathbf{x}, 0) = \mathbf{u}_{0h}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \overline{B_h(0)}, \tag{2.4.35}$$

$$\left\langle \boldsymbol{\mu}_h, \mathbf{u}_h(t) - \mathbf{V}(t) - \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G}(\mathbf{t})\mathbf{x}} \right\rangle_{\Lambda_h(t)} = 0, \forall \boldsymbol{\mu}_h \in \Lambda_h(t), \tag{2.4.36}$$

$$\mathbf{G}(\mathbf{x}, 0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x}, 0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x}, 0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{2.4.37}$$

where $\mathbf{u}_{0h}$ is an approximation of $\mathbf{u}_0$ such that

$$\int_\Omega q\nabla \cdot \mathbf{u}_{0h} \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L_h^2.$$

2.4.2 Collocation Boundary Method and Immersed Boundary Method

When we deal with the boundary of the particle $B(t)$, there are several methods have been considered for discretization. Here we introduce two of them, which are collocation boundary method and immersed boundary method.

For collocation boundary method, we define the scalar pairing $< \cdot, \cdot >_{\Lambda_h(t)}$ as follows:

$$\langle \boldsymbol{\mu}_h, \mathbf{v}_h \rangle_{\Lambda_h(t)} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \cdot \mathbf{v}_h(\mathbf{x}_i), \;\; \forall \boldsymbol{\mu}_h \in \Lambda_h(t), \mathbf{v}_h \in \mathbf{V}_{\mathbf{g}_{0h}(t)} \text{ or } \mathbf{V}_{0h},$$

By using the above scalar pairing $< \cdot, \cdot >_{B_h(t)}$, the rigid body motion of particle $B(t)$ is forced via a collocation boundary method.

For immersed boundary method, we define the scalar pairing $< \cdot, \cdot >_{\Lambda_h(t)}$ as follows:

$$\langle \boldsymbol{\mu}_h, \mathbf{v}_h \rangle_{\Lambda_h(t)} = \sum_{i=1}^{N} \sum_{j=1}^{M} \boldsymbol{\mu}_i \cdot \mathbf{v}_h(\mathbf{x}_j) D_h(\mathbf{x}_j - \xi_i) h^3, \;\; \forall \boldsymbol{\mu}_h \in \Lambda_h(t), \mathbf{v}_h \in \mathbf{V}_{\mathbf{g}_{0h}(t)} \text{ or } \mathbf{V}_{0h},$$

where $\{\mathbf{x}_j\}_{j=1}^{M}$ are the grid points of the finite elements for the velocity, and the function $D_h(\mathbf{X} - \xi_i)$ is defined as

$$D_h(\mathbf{X} - \xi_i) = \delta_h(X_1 - \xi_{i1})\delta_h(X_2 - \xi_{i2})\delta_h(X_3 - \xi_{i3})$$

with $\mathbf{X} = (X_1, X_2, X_3)$ and $\xi_i = (\xi_{i1}, \xi_{i2}, \xi_{i3})$, and the one-dimensional discrete δ_h defined by

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

By using the above scalar pairing $< \cdot, \cdot >_{\Lambda_h(t)}$, the rigid body motion of particle $B(t)$ is forced via an immersed boundary method.

2.4.3 Operator Splitting scheme

Applying the Lie's scheme to the discrete analogue of the problem (2.3.26)-(2.4.37) and backward Euler's method, we obtain:

Given $\mathbf{u}^0 = \mathbf{u}_{0h}, \mathbf{G}^0 = \mathbf{G}_0, \mathbf{V}^0 = \mathbf{V}_0, \boldsymbol{\omega}^0 = \boldsymbol{\omega}_0$. For $n \geq 0$, $\mathbf{u}^n, \mathbf{G}^n, \mathbf{V}^n, \boldsymbol{\omega}^n$ are known, we predict the position and the translation velocity of the center of mass as follows.

$$\frac{d\mathbf{G}}{dt} = \mathbf{V}(t), \tag{2.4.38}$$

$$M_p \frac{d\mathbf{V}}{dt} = \mathbf{0}, \tag{2.4.39}$$

$$\mathbf{I_p} \frac{d\boldsymbol{\omega}}{dt} = \mathbf{0}, \tag{2.4.40}$$

$$\mathbf{V}(t^n) = \mathbf{V}^n, \boldsymbol{\omega}(t^n) = \boldsymbol{\omega}^n, \mathbf{G}(t^n) = \mathbf{G}^n, \tag{2.4.41}$$

for $t^n < t < t^{n+1}$. Then set $\mathbf{V}^{n+\frac{1}{2}} = \mathbf{V}(t^{n+1})$, $\boldsymbol{\omega}^{n+\frac{1}{2}} = \boldsymbol{\omega}(t^{n+1})$, and $\mathbf{G}^{n+\frac{1}{2}} = \mathbf{G}(t^{n+1})$.

and we get $B_h^{n+\frac{1}{2}}$ based on the center of particle $\mathbf{G}^{n+\frac{1}{2}}$ and take $\boldsymbol{\omega}^{n+\frac{1}{2}} = \boldsymbol{\omega}^n$.

Then we enforce the rigid body motion in $B_h^{n+\frac{1}{2}}$ and solve $\mathbf{u}^{n+1}$ and p^{n+1} simultaneously as follows:

Find $\mathbf{u}^{n+1} \in \mathbf{V}_{\mathbf{g}_{0h}}^{n+1}$, $p^{n+1} \in L_{0h}^2$, $\boldsymbol{\lambda}^{n+1} \in \Lambda_h^{n+1}$, $\mathbf{V}^{n+1} \in \mathbb{R}^3$, $\boldsymbol{\omega}^{n+1} \in \mathbb{R}^3$ such that

$$\begin{cases} -\displaystyle\int_\Omega p^{n+1} \nabla \cdot \mathbf{v}\, \mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \nabla \mathbf{u}^{n+1} : \nabla \mathbf{v}\, \mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathbf{V}^{n+1} - \mathbf{V}^{n+\frac{1}{2}}}{\Delta t} \cdot \mathbf{Y} + \mathbf{I}_p \dfrac{\boldsymbol{\omega}^{n+1} - \boldsymbol{\omega}^{n+\frac{1}{2}}}{\Delta t} \cdot \boldsymbol{\theta} \\ = \left(1 - \dfrac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} + \left\langle \boldsymbol{\lambda}^{n+1}, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}^{n+\frac{1}{2}}\mathbf{x}} \right\rangle_{\Lambda_h^{n+1}}, \\ \forall\ (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{V}_{0h} \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{2.4.42}$$

$$\int_\Omega q \nabla \cdot \mathbf{u}^{n+1}\, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L_h^2, \tag{2.4.43}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u}^{n+1} - \mathbf{V}^{n+1} - \boldsymbol{\omega}^{n+1} \times \overrightarrow{\mathbf{G}^{n+\frac{1}{2}}\mathbf{x}} \right\rangle_{\Lambda_h^{n+1}} = 0, \quad \forall \boldsymbol{\mu} \in \Lambda_h^{n+\frac{1}{2}}. \tag{2.4.44}$$

Finally we set $\mathbf{G}^{n+1} = \mathbf{G}^{n+\frac{1}{2}}$.

In the above, $\mathbf{V}_{\mathbf{g}_{0h}}^{n+1} = \mathbf{V}_{\mathbf{g}_{0h}(t^{n+1})}$, $\Lambda_h^{n+1} = \Lambda_h(t^{n+1})$, and $B_h^{n+s} = B_h(t^{n+s})$.

2.5 On the solution of the subproblems from operator splitting

2.5.1 Solution of the rigid body motion enforcement problems

In system (2.4.42)-(2.4.44), there are two multipliers. p and $\boldsymbol{\lambda}$. We have solved this system via an Uzawa-conjugate gradient method driven by both multipliers. The general problem is as follows:

Find $\mathbf{u} \in \mathbf{V}_{\mathbf{g}_{0h}}$, $p \in L^2_{0h}$, $\boldsymbol{\lambda} \in \Lambda_h$, $\mathbf{V} \in \mathbb{R}^3$, $\boldsymbol{\omega} \in \mathbb{R}^3$ such that

$$\begin{cases} -\int_\Omega p\nabla\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + \mu_f \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\,\mathrm{d}\mathbf{x} + M_p \dfrac{\mathbf{V}-\mathbf{V}_0}{\triangle t}\cdot\mathbf{Y} + \mathbf{I_p}\dfrac{\boldsymbol{\omega}-\boldsymbol{\omega}_0}{\triangle t}\cdot\boldsymbol{\theta} \\ = \left(1-\dfrac{\rho_f}{\rho_s}\right) M_p\mathbf{g}\cdot\mathbf{Y} + \left\langle \boldsymbol{\lambda}, \mathbf{v}-\mathbf{Y}-\boldsymbol{\theta}\times\overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \\ \forall\ (\mathbf{v},\mathbf{Y},\boldsymbol{\theta}) \in \mathbf{V}_{0h}\times\mathbb{R}^3\times\mathbb{R}^3, \end{cases} \tag{2.5.45}$$

$$\int_\Omega q\nabla\cdot\mathbf{u}\,\mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2_h, \tag{2.5.46}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u}-\mathbf{V}-\boldsymbol{\omega}\times\overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h} = 0, \quad \forall\boldsymbol{\mu} \in \Lambda_h. \tag{2.5.47}$$

Applying the following Uzawa-conjugate gradient algorithm operating in the space $L^2_{0h}\times\Lambda_h$ to solve the sysyem (2.5.45)-(2.5.47):

Assume $p^0 \in L^2_{0h}$ and $\boldsymbol{\lambda}^0 \in \Lambda_h$ are given.

We solve the problem:

Find $\mathbf{u}^0 \in \mathbf{V}_{\mathbf{g}_{0h}}$, $\mathbf{V}^0 \in \mathbb{R}^3$, $\boldsymbol{\omega}^0 \in \mathbb{R}^3$ *satisfying*

$$\begin{cases} \mu_f \int_\Omega \nabla \mathbf{u}^0 : \nabla \mathbf{v}\, d\mathbf{x} = \int_\Omega p \nabla \cdot \mathbf{v}\, d\mathbf{x} + \left\langle \boldsymbol{\lambda}^0, \mathbf{v} \right\rangle_{\Lambda_h}, \\ \forall\ \mathbf{v} \in \mathbf{V}_{0h}; \mathbf{u}^0 \in \mathbf{V}_{\mathbf{g}_{0h}}, \end{cases} \tag{2.5.48}$$

$$M_p \frac{\mathbf{V}^0 - \mathbf{V}_0}{\triangle t} \cdot \mathbf{Y} = \left(1 - \frac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} - \left\langle \boldsymbol{\lambda}^0, \mathbf{Y} \right\rangle_{\Lambda_h}, \quad \forall\ \mathbf{Y} \in \mathbb{R}^3, \tag{2.5.49}$$

$$\mathbf{I_p} \frac{\boldsymbol{\omega}^0 - \boldsymbol{\omega}_0}{\triangle t} \cdot \boldsymbol{\theta} = -\left\langle \boldsymbol{\lambda}^0, \boldsymbol{\theta} \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\theta} \in \mathbb{R}^3, \tag{2.5.50}$$

and then compute

$$\mathrm{g}_1^0 = \nabla \cdot \mathbf{u}^0; \tag{2.5.51}$$

next find $\mathbf{g}_2^0 \in \Lambda_h$ *satisfying*

$$\left\langle \boldsymbol{\mu}, \mathbf{g}_2^0 \right\rangle_{\Lambda_h} = \left\langle \boldsymbol{\mu}, \mathbf{u}^0 - \mathbf{V}^0 - \boldsymbol{\omega}^0 \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\mu} \in \Lambda_h, \tag{2.5.52}$$

and set

$$\mathrm{w}_1^0 = \mathrm{g}_1^0, \quad \mathbf{w}_2^0 = \mathbf{g}_2^0. \tag{2.5.53}$$

Then for $k \geq 0$, *assuming that* p^k, $\boldsymbol{\lambda}^k$, $\mathbf{u}^k$, $\mathbf{V}^k$, $\boldsymbol{\omega}^k$, $\mathrm{g}_1^{\mathrm{k}}$, $\mathbf{g}_2^k$, w_1^k *and* $\mathbf{w}_2^k$ *are known, compute* p^{k+1}, $\boldsymbol{\lambda}^{k+1}$, $\mathbf{u}^{k+1}$, $\mathbf{V}^{k+1}$, $\boldsymbol{\omega}^{k+1}$, $\mathrm{g}_1^{\mathrm{k+1}}$, $\mathbf{g}_2^{k+1}$, ${\mathrm{w}_1}^{k+1}$ *and* $\mathbf{w}_2^{k+1}$ *as follows:*

$$\begin{cases} \mu_f \int_\Omega \nabla \overline{\mathbf{u}}^k : \nabla \mathbf{v}\, d\mathbf{x} = \int_\Omega \mathrm{w}_1^k \nabla \cdot \mathbf{v}\, d\mathbf{x} + \left\langle \mathbf{w}_2^k, \mathbf{v} \right\rangle_{\Lambda_h}, \\ \forall\ \mathbf{v} \in \mathbf{V}_{0h}; \overline{\mathbf{u}}^k \in \mathbf{V}_{\mathbf{g}_{0h}}, \end{cases} \tag{2.5.54}$$

$$M_p \frac{\overline{\mathbf{V}}^k}{\triangle t} \cdot \mathbf{Y} = -\left\langle \mathbf{w}_2^k, \mathbf{Y} \right\rangle_{\Lambda_h}, \quad \forall\ \mathbf{Y} \in \mathbb{R}^3, \tag{2.5.55}$$

$$\mathbf{I_p} \frac{\overline{\boldsymbol{\omega}}^k}{\triangle t} \cdot \boldsymbol{\theta} = -\left\langle \mathbf{w}_2^k, \boldsymbol{\theta} \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\theta} \in \mathbb{R}^3, \tag{2.5.56}$$

and then compute

$$\overline{\mathrm{g}}_1^{\mathrm{k}} = \nabla \cdot \overline{\mathbf{u}}^{\mathrm{k}}; \tag{2.5.57}$$

next find $\overline{\mathbf{g}}_2^k \in \Lambda_h$ *satisfying*

$$\left\langle \boldsymbol{\mu}, \overline{\mathbf{g}}_2^k \right\rangle_{\Lambda_h} = \left\langle \boldsymbol{\mu}, \overline{\mathbf{u}}^k - \overline{\mathbf{V}}^k - \overline{\boldsymbol{\omega}}^k \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\mu} \in \Lambda_h, \tag{2.5.58}$$

and compute

$$\rho_k = \frac{\displaystyle\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^k, \mathbf{g}_2^k \right\rangle_{\Lambda_h}}{\displaystyle\int_\Omega \overline{\mathbf{g}}_1^k \mathrm{w}_1^k \, d\mathbf{x} + \left\langle \overline{\mathbf{g}}_2^k, \mathbf{w}_2^k \right\rangle_{\Lambda_h}}, \tag{2.5.59}$$

and

$$p^{k+1} = p^k - \rho_k {\mathrm{w}_1}^k, \tag{2.5.60}$$

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k - \rho_k \mathbf{w}_2^k, \tag{2.5.61}$$

$$\mathbf{u}^{k+1} = \mathbf{u}^k - \rho_k \overline{\mathbf{u}}^k, \tag{2.5.62}$$

$$\mathbf{V}^{k+1} = \mathbf{V}^k - \rho_k \overline{\mathbf{V}}^k, \tag{2.5.63}$$

$$\boldsymbol{\omega}^{k+1} = \boldsymbol{\omega}^k - \rho_k \overline{\boldsymbol{\omega}}^k, \tag{2.5.64}$$

$$\mathrm{g}_1^{k+1} = \mathrm{g}_1^k - \rho_k \overline{\mathrm{g}}_1^k, \tag{2.5.65}$$

$$\mathbf{g}_2^{k+1} = \mathbf{g}_2^k - \rho_k \overline{\mathbf{g}}_2^k. \tag{2.5.66}$$

If

$$\frac{\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}+1}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{k+1}, \mathbf{g}_2^{k+1} \right\rangle_{\Lambda_h}}{\int_\Omega \left|\mathrm{g}_1^0\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^0, \mathbf{g}_2^0 \right\rangle_{\Lambda_h}} \leq \varepsilon, \tag{2.5.67}$$

then take $p = p^{k+1}$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}^{k+1}$, $\mathbf{u} = \mathbf{u}^{k+1}$, $\mathbf{V} = \mathbf{V}^{k+1}$, *and* $\boldsymbol{\omega} = \boldsymbol{\omega}^{k+1}$. *Otherwise, compute*

$$\gamma_k = \frac{\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}+1}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{k+1}, \mathbf{g}_2^{k+1} \right\rangle_{\Lambda_h}}{\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^k, \mathbf{g}_2^k \right\rangle_{\Lambda_h}}, \tag{2.5.68}$$

and set

$$\mathrm{w}_1^{k+1} = \mathrm{g}_1^{k+1} + \gamma_k {\mathrm{w}_1}^k, \tag{2.5.69}$$

$$\mathbf{w}_2^{k+1} = \mathbf{g}_2^{k+1} + \gamma_k \mathbf{w}_2^k. \tag{2.5.70}$$

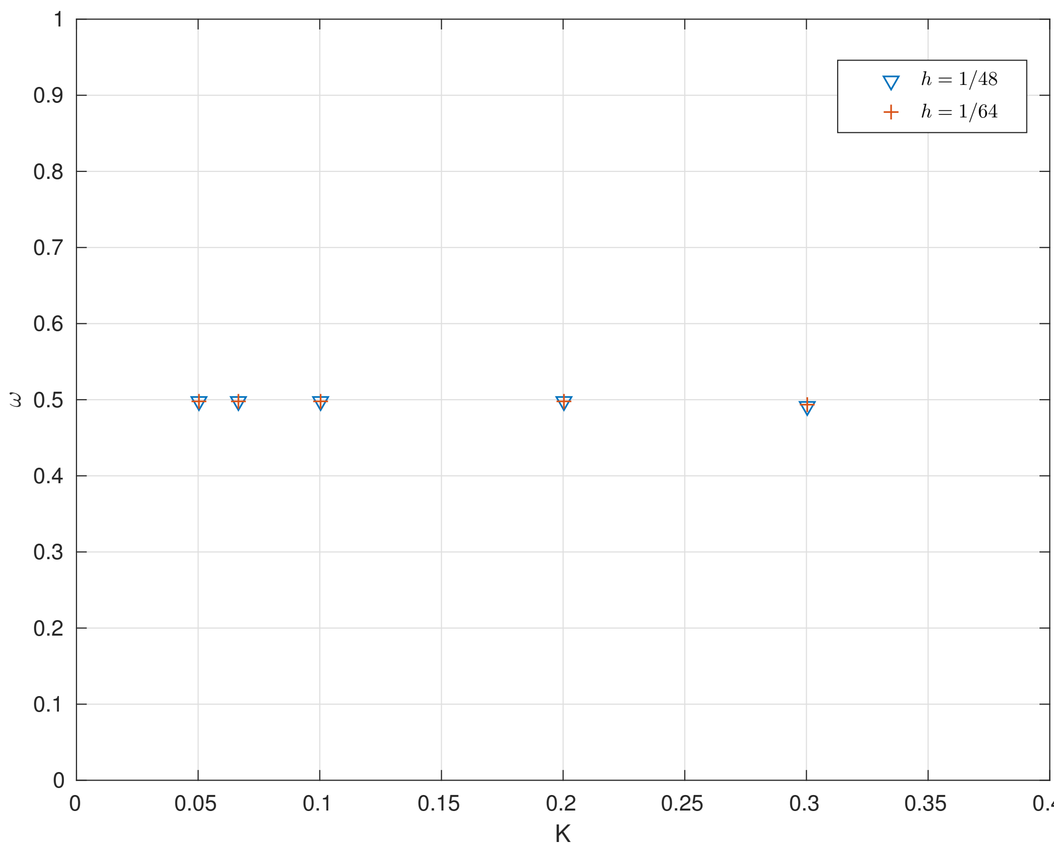
Then do $m = m + 1$ *and go back to* (2.5.54).

2.6 Numerical results

2.6.1 Rotation of a single particle

We have first considered the cases of a single neutrally buoyant ball in a bounded shear flow of a Newtonian fluid. The ball is placed at the middle between two walls initially, and it remains there in simulation even though it can move freely in fluid. The computational domain is $\Omega = (-1, 1) \times (-1, 1) \times (-H/2, H/2)$ (i.e., $L_1 = 2$ and $L_2 = 2$) for different values of the height H. The ball radius is $a = 0.15$ and its mass center is located at (0,0,0) initially. The blockage ratio is defined by $K = 2a/H$.

The shear rate $\dot{\gamma} = 1$ so the velocity of the top wall is $U = H/2$ and that of the bottom wall is $-U = -H/2$. The fluid and particle densities are $\rho_f = \rho_s = 1$, the fluid viscosity being $\mu = 1$. The mesh sizes for the velocity field is $h = 1/48$ or $1/64$ and the mesh size for the pressure is $2h$, the time step being $\Delta t = 0.001$. For all the numerical simulations considered in this section, we assume that all dimensional quantities are in the CGS units.



Under creeping conditions, the rotating velocity of the ball with respect to the x_2-axis (see Fig. **??**) is $\dot{\gamma}/2 = 0.5$ in an unbounded shear flow of a Newtonian fluid, according to the associated Jeffery's solution [10]. In Fig. **??**, the ball rotating velocities have been shown for different values of the blockage ratio. Our numerical results are in a good agreement with the Jeffery's solution for most values of the blockage ratio; but we can observe the wall influence on the rotating velocity for the largest value of the blockage ratio, $K = 0.3$, in Fig. **??**.

2.6.2 Sedimentation of a single particle

In this section we have considered the terminal speed of sedimentary single particle in a vertical channel of infinitie length fillled with a Newtonian fluid. The computational domain is $\Omega = (-1, 1) \times (-1, 1) \times (-1, 1)$. The ball radius is $a = 0.1$ and its mass center is located at (0,0,0) initially. The fluid and particle densities are $\rho_f = 1$,$\rho_s = 1.5$, the fluid viscosity being $\mu = 1$. The mesh sizes for the velocity field is $h = 1/48$, $1/64$, or $1/80$ and the mesh size for the pressure is $2h$, the time step being $\Delta t = 0.001$. We can valid the numerical results with the theoretical solution in [**?**, 7]. The formula of the theoretical solution of terminal speed V of sedimentary single particle is

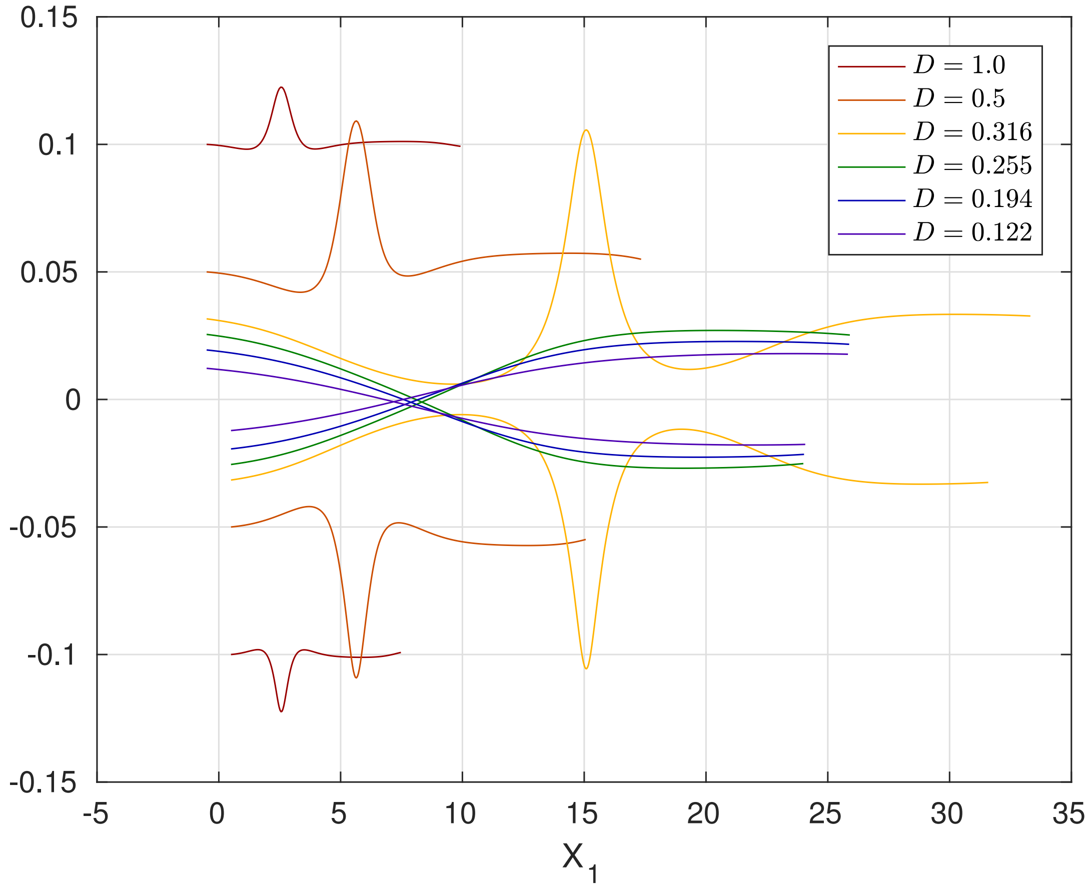
$$V = \frac{2}{9}\frac{\rho_s - \rho_f}{\mu} g a^2 \tag{2.6.71}$$

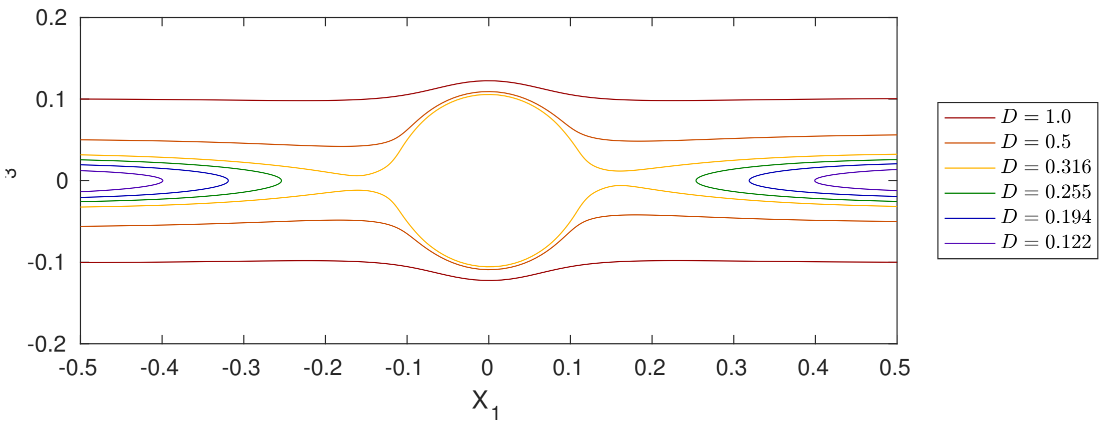
where g is the gravity. So the theoretical solution in our case is -1.0896.

Mesh Size H	Terminal Speed	
	Collocation Boundary Method	Immersed Boundary Method
1/48	-1.0147	-0.9495
1/64	-1.0558	-0.9919
1/80	-1.0662	-1.0151

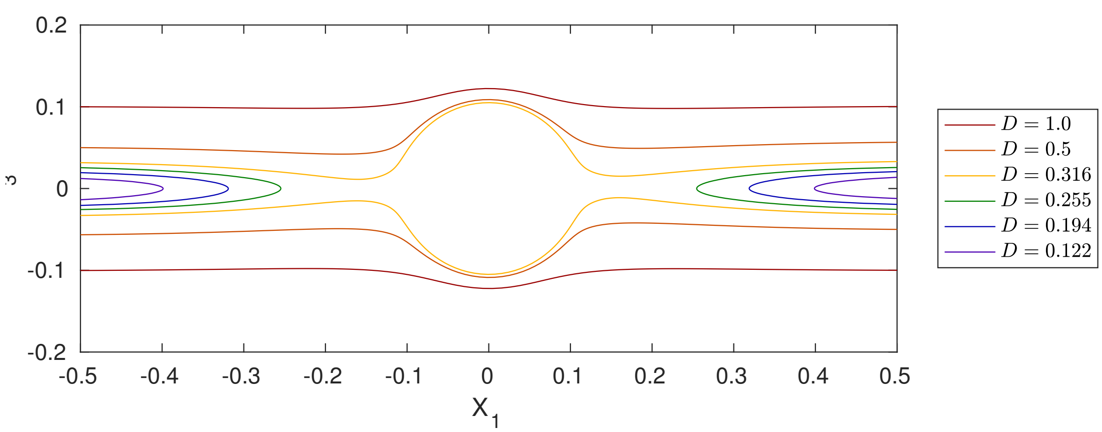
Table 2.6.1

2.6.3 Two balls interaction in an one wall-driven bounded shear flow





2.6.4 Two balls interaction in a two wall-driven bounded shear flow



CHAPTER 3

3D DLM/FD methods for simulating the motion of spheres in bounded shear flows of Oldroyd-B fluids

3.1 Several Models of Non-Newtonian Fluid

3.1.1 Stokes Equations

Consider the Stokes equations in $\Omega \times (0, T)$ describing the 3-dimensional motion of an incompressible and isothermal fluid without body force:

$$\begin{cases} -\nabla \cdot \sigma = \rho_f \mathbf{g}, \\ \nabla \cdot \mathbf{u} = 0. \end{cases}$$

where $\sigma = -p\mathbf{I} + \boldsymbol{\tau}$ with presure p and stress tensor $\boldsymbol{\tau}$, $\mathbf{u} = (u_1, u_2, u_3)$ is the flow velocity, $\mathbf{g}$ is the gravity, and ρ_f is the density of fluid.

3.1.2 Newtonian Model

The constitutive equation of the stress tensor is given by

$$\boldsymbol{\tau} = 2\mu\mathbf{D}(\mathbf{u})$$

where μ is the solvent viscosity of the fluid and $\mathbf{D}(\mathbf{u})$ is the symmetric rate of strain tensor

$$2\mathbf{D}(\mathbf{u}) = \nabla\mathbf{u} + (\nabla\mathbf{u})^t,$$

with the Jacobian of the velocity $\nabla\mathbf{u}$.

3.1.3 The UCM-model

In the UCM-model, we use the following constitutive equation to describe the viscoelastic stress tensor $\boldsymbol{\tau}_E$:

$$\lambda_1\overset{\triangledown}{\boldsymbol{\tau}}_E + \boldsymbol{\tau}_E = 2\eta\mathbf{D}(\mathbf{u}).$$

Here $\overset{\triangledown}{\boldsymbol{\tau}}_E$ is called the upper-convected time derivative of $\boldsymbol{\tau}_E$ and is defined by

$$\overset{\triangledown}{\boldsymbol{\tau}}_E = \frac{\partial\boldsymbol{\tau}_E}{\partial t} + (\mathbf{u}\cdot\nabla)\boldsymbol{\tau}_E - \boldsymbol{\tau}_E\cdot(\nabla\mathbf{u})^t - (\nabla\mathbf{u})\cdot\boldsymbol{\tau}_E,$$

where λ_1 is the relaxation time of the fluid, and η is the elastic viscosity of the fluid.

So we have the constitutive equation

$$\frac{\partial \boldsymbol{\tau}_E}{\partial t} + (\mathbf{u} \cdot \nabla)\boldsymbol{\tau}_E - \boldsymbol{\tau}_E \cdot (\nabla \mathbf{u})^t - (\nabla \mathbf{u}) \cdot \boldsymbol{\tau}_E + \frac{1}{\lambda_1}\boldsymbol{\tau}_E = \frac{2\eta}{\lambda_1}\mathbf{D}(\mathbf{u}).$$

3.1.4 The Oldroyd-B model

In the more general Oldroyd-B model, the stress tensor $\boldsymbol{\tau}$ is composed of a Newtonian component $\boldsymbol{\tau}_s$ and a viscoelastic component $\boldsymbol{\tau}_E$,

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_E,$$

and $\boldsymbol{\tau}_s$ is governed by a Newtonian consitutive equation $\boldsymbol{\tau}_s = 2\mu\mathbf{D}(\mathbf{u})$.

Thus, the Oldroyd-B model can be seen as a linear interpolation of the UCM and the Newtonian model:

$$\begin{cases} -\nabla \cdot \sigma = \rho_f \mathbf{g}, \\ \nabla \cdot \mathbf{u} = 0, \\ \lambda_1 \overset{\nabla}{\boldsymbol{\tau}}_E + \boldsymbol{\tau}_E = 2\eta\mathbf{D}(\mathbf{u}), \end{cases}$$

where $\sigma = -p\mathbf{I} + \boldsymbol{\tau}_s + \boldsymbol{\tau}_E$.

Using $\sigma = -p\mathbf{I} + 2\mu\mathbf{D}(\mathbf{u}) + \boldsymbol{\tau}_E$, we obtain

$$\nabla p - 2\mu\nabla \cdot \mathbf{D}(\mathbf{u}) - \nabla \cdot \boldsymbol{\tau}_E = \rho_f \mathbf{g}.$$

Remark 3.1. *Using the definition of conformation tenser* $\mathbf{C} = \dfrac{\lambda_1}{\eta}\boldsymbol{\tau}_E + \mathbf{I}$, *we obtain* *the Oldroyd-B model in terms of* $\mathbf{C}$*:*

$$\begin{cases} \nabla p - 2\mu\nabla\cdot\mathbf{D}(\mathbf{u}) - \dfrac{\eta}{\lambda_1}\nabla\cdot(\mathbf{C}-\mathbf{I}) = \rho_f\mathbf{g}, \\ \nabla\cdot\mathbf{u} = 0, \\ \dfrac{\partial\mathbf{C}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{C} - (\nabla\mathbf{u})\cdot\mathbf{C} - \mathbf{C}\cdot(\nabla\mathbf{u})^t + \dfrac{1}{\lambda_1}\mathbf{C} = \dfrac{1}{\lambda_1}\mathbf{I}, \end{cases}$$

where λ_1 *is the relaxation time of the fluid,* η *is the elastic viscosity of the fluid, and* $\mathbf{I}$ *is the identity matrix. Here the conformation tensor* $\mathbf{C}$ *is symmetric and positive definite.*

3.1.5 The Carreau model

We also consider the non-Newtonian fluid with shear thinning. In pure Oldroyd-B Model, the viscosity of fluid η_1 is a constant on the given domain and we define the elastic viscosity of the fluid η to be

$$\eta = \eta_1\left(1 - \frac{\lambda_2}{\lambda_1}\right)$$

where λ_1 is relaxation time and λ_2 is retardation time.

To consider the shear thinning in Oldroyd-B model, we use Carreau model to simulate it. Under Carreau model, the viscosity of fluid $\eta_1(\dot{\gamma_e})$ depends on the fluid velocity. We define $\eta_1(\dot{\gamma_e})$ to be

$$\eta_1(\dot{\gamma_e}) = \frac{\eta_1}{\left(1 + (\lambda_1\dot{\gamma_e})^2\right)^{\frac{1-n}{2}}} \tag{3.1.1}$$

where η_1 is the fluid viscosity without shear thinning, $\dot{\gamma}_e = \sqrt{2\mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{u})}$ and n is a number less than 1.

3.2 DLM/FD method for simulating fluid-particle interaction in stokes flow

3.2.1 The governing equations

Let Ω be a bounded domain in $\mathbb{R}^3$ and let Γ be the boundary of Ω. We suppose that Ω is filled with a viscoelasic fluid of Oldroyd-B type with density ρ_f and contains N moving particles of density ρ_s. Let $B(t) = \overset{N}{\underset{i=1}{\cup}} B_i(t)$ where $B_i(t)$ is the i-th solid particle in the fluid for $i = 1, 2, \cdots, N$. We denote by $\gamma_i(t)$ the boundary $\partial B_i(t)$ of $B_i(t)$ for $i = 1, 2, \cdots, N$ and let $\gamma(t) = \overset{N}{\underset{i=1}{\cup}} \gamma_i(t)$.

For some $T > 0$, the governing equations for the fluid-particles system is as follows:

For the motion of fluid, we consider the Stokes equations in Oldroyd-B model

$$\nabla p - 2\mu \nabla \cdot \mathbf{D}(\mathbf{u}) - \frac{\eta}{\lambda_1} \nabla \cdot (\mathbf{C} - \mathbf{I}) = \rho_f \mathbf{g} \quad \text{in } \Omega \setminus \overline{B(t)}, t \in (0, T), \tag{3.2.2}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \setminus \overline{B(t)}, t \in (0, T), \tag{3.2.3}$$

$$\mathbf{u} = \mathbf{g_0} \quad \text{on } \Gamma \times (0, T), \text{with } \int_\Gamma \mathbf{g_0} \cdot \mathbf{n} d\Gamma = 0, \tag{3.2.4}$$

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{V}_i(t) + \boldsymbol{\omega}_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \mathbf{x} \in \gamma_i(t),\ i = 1, 2, \cdots, N, \tag{3.2.5}$$

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{C} - (\nabla \mathbf{u}) \cdot \mathbf{C} - \mathbf{C} \cdot (\nabla \mathbf{u})^t + \frac{1}{\lambda_1}\mathbf{C} = \frac{1}{\lambda_1}\mathbf{I} \quad \text{in } \Omega \setminus \overline{B(t)}, t \in (0,T), \tag{3.2.6}$$

$$\mathbf{C}(\mathbf{x}, 0) = \mathbf{C}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega \setminus \overline{B(0)}, \tag{3.2.7}$$

$$\mathbf{C} = \mathbf{C}_L \quad \text{on } \Gamma^-, \tag{3.2.8}$$

where $\mathbf{n}$ is the unit normal vector pointing outward to the flow region.

In (3.2.5), we assume a no-slip condition on the boundary of particles $\gamma(t)$

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{V}_i(t) + \boldsymbol{\omega}_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \mathbf{x} \in \gamma_i(t),\ i = 1, 2, \cdots, N,$$

where $\mathbf{V}_i$ is the translation velocity, $\boldsymbol{\omega}_i$ is the angular velocity, $\mathbf{G_i}$ is the center of mass and $\mathbf{x}$ is a point on the surface of the particle.

The motion of particle satisfies the Euler-Newton's equations

$$\mathbf{v}_i(\mathbf{x}, t) = \mathbf{V}_i(t) + \boldsymbol{\omega}_i(t) \times \overrightarrow{\mathbf{G}_i(t)\mathbf{x}}, \quad \forall \{\mathbf{x}, t\} \in \overline{B_i(t)} \times (0, T),\ i = 1, 2, \cdots, N, \tag{3.2.9}$$

$$\frac{\mathrm{d}\mathbf{G}_i}{\mathrm{d}t} = \mathbf{V}_i, \tag{3.2.10}$$

$$M_i \frac{\mathrm{d}\mathbf{V_i}}{\mathrm{d}t} = M_i \mathbf{g} + \mathbf{F}_i + \mathbf{F}_i^r, \tag{3.2.11}$$

$$\frac{\mathrm{d}(\boldsymbol{I}_i \boldsymbol{\omega}_i)}{\mathrm{d}t} = \mathbf{T}_i + \overrightarrow{\mathbf{G}_i \mathbf{x}_r} \times \mathbf{F}_i^r, \tag{3.2.12}$$

$$\mathbf{G}_i(0) = \mathbf{G}_i^0,\ \mathbf{V}_i(0) = \mathbf{V}_i^0,\ \boldsymbol{\omega}_i(0) = \boldsymbol{\omega}_i^0, \tag{3.2.13}$$

for $i = 1, 2, \cdots, N$, where M_i and I_i are the mass and the moment of inertia of the i-th particle, respectively; $\mathbf{F}_i$ and $\mathbf{T}_i$ are the hydrodynamical force and torque imposed on the i-th particle by the fluid, and $\mathbf{F}_i^r$ is a short range repulsion force imposed on the i-th particle by other particles and wall to prevent particle/particle and particle/wall penetration.

The hydrodynamical force $\mathbf{F}_i$ and torque $\mathbf{T}_i$ imposed on the i-th particle by the fluid are given by

$$\mathbf{F}_i = -\int_\gamma \sigma \mathbf{n}\, \mathrm{d}\gamma, \quad \mathbf{T}_i = -\int_\gamma \overrightarrow{\mathbf{G}_i\mathbf{x}} \times \sigma \mathbf{n}\, \mathrm{d}\gamma. \tag{3.2.14}$$

$\overrightarrow{\mathbf{G}_i\mathbf{x}_r} \times \mathbf{F}_i^r$ is a torque acting on the point $\mathbf{x}_r$ where $\mathbf{F}_i^r$ applies on the i-th particle.

3.2.2 DLM/FD formulation

To obtain a distributed Lagrange multiplier/ fictitious domain formulation for the above problem (3.2.2) – (3.2.14), we have the following three steps, namely: (i) we derive a global variational formulation of the virtual power type of problem (3.2.2) – (3.2.14), (ii) we then extend the fluid motion into the region of particles with rigid body motion constraint, and then (iii) we relax that constraint by using a distributed lagrange multiplier.

For convenience of derivation, we assume there is only one particle in the fluid, that is, we set $B(t)$ the solid particle in the fluid, $\gamma(t)$ the boundary $\partial B(t)$ of $B(t)$, $\mathbf{G}(t)$ the center of mass of this particle. In the equations of the motion of particle, we set $\mathbf{V}$ the translation velocity of the particle $B(t)$, $\boldsymbol{\omega}$ the angular velocity of the particle $B(t)$, M_p and $\mathbf{I_p}$ the mass and the moment of inertia of the particle $B(t)$, respectively; $\mathbf{F}$ and $\mathbf{T}$ the hydrodynamical force and torque imposed on the particle $B(t)$ by the fluid, respectively, and $\mathbf{F}^r$ a short range repulsion force imposed on the particle $B(t)$.

To obtain a variational formulation for above problem (3.2.2) – (3.2.8), we define the following function spaces

$$\mathbf{W}_{\mathbf{g}_0}(t) = \left\{ \mathbf{v} \,\middle|\, \mathbf{v} \in (H^1(\Omega \setminus \overline{B(t)}))^3, \mathbf{v} = \mathbf{g}_0(t) \,\text{on}\, \Gamma, \mathbf{v} = \mathbf{V}(t) + \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \text{on } \partial B(t) \right\},$$

$$\mathbf{W}_0(t) = \left\{ (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \,\middle|\, \mathbf{v} \in (H^1(\Omega \setminus \overline{B(t)}))^3, \mathbf{v} = 0 \text{ on}\, \Gamma, \mathbf{v} = \mathbf{Y} + \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \text{on } \partial B(t), \;\; \text{with } \mathbf{Y} \in \mathbb{R}$$

$$L^2_0(\Omega \setminus \overline{B(t)}) = \left\{ q \,\middle|\, q \in L^2(\Omega \setminus \overline{B(t)}), \int_{\Omega \setminus \overline{B(t)}} q \,\mathrm{d}\mathbf{x} = 0 \right\},$$

and

$$\mathbf{W}(\Omega \setminus \overline{B(t)}) = \left\{ \mathbf{A} \,\middle|\, \mathbf{A} = [a_{ij}] \in M_{3\times 3}, a_{ij} \in H^1(\Omega \setminus \overline{B(t)}), i, j = 1, 2, 3 \right\},$$

$$\mathbf{W}_{\mathbf{C}_L}(\Omega \setminus \overline{B(t)}) = \left\{ \mathbf{A} \,\middle|\, \mathbf{A} \in \mathbf{W}(\Omega \setminus \overline{B(t)}), \mathbf{A} = \mathbf{C}_L(t) \,\text{on}\, \Gamma^- \right\}.$$

Applying the virtual power principle to the system (3.2.2) – (3.2.8) obtains the following variational formulation:

For a.e. $t \in (0, T)$, find $\mathbf{u}(t) \in \mathbf{W}_{\mathbf{g}_0}(t)$, $p(t) \in L^2_0(\Omega \setminus \overline{B(t)})$, $\mathbf{C}(t) \in \mathbf{W}_{\mathbf{C}_L}$,$\mathbf{V}(t) \in$

$\mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, such that

$$\begin{cases} -\displaystyle\int_{\Omega\setminus\overline{B(t)}} p\nabla\cdot\mathbf{v}\mathrm{d}\mathbf{x} + 2\mu_f \int_{\Omega\setminus\overline{B(t)}} \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\mathrm{d}\mathbf{x} \\ -\dfrac{\eta}{\lambda_1}\displaystyle\int_{\Omega\setminus\overline{B(t)}} \mathbf{v}\cdot(\nabla\cdot(\mathbf{C}-\mathbf{I}))\mathrm{d}\mathbf{x} + \left(M_p\dfrac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} - M_p\mathbf{g} - \mathbf{F}^r\right)\cdot\mathbf{Y} \\ +\left(\dfrac{\mathrm{d}\left(\mathbf{I_p}\boldsymbol{\omega}\right)}{\mathrm{d}t} - \overrightarrow{\mathbf{Gx}_r}\times\mathbf{F}^r\right)\cdot\boldsymbol{\theta} = \rho_f\displaystyle\int_{\Omega\setminus\overline{B(t)}} \mathbf{g}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} \quad \forall(\mathbf{v},\mathbf{Y},\boldsymbol{\theta})\in\mathbf{W}_0(t), \end{cases} \tag{3.2.15}$$

$$\int_{\Omega\setminus\overline{B(t)}} q\nabla\cdot\mathbf{u}\,\mathrm{d}\mathbf{x} = 0, \quad \forall q\in L^2(\Omega\setminus\overline{B(t)}), \tag{3.2.16}$$

$$\begin{cases} \displaystyle\int_{\Omega\setminus\overline{B(t)}} \left(\frac{\partial\mathbf{C}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{C} - (\nabla\mathbf{u})\cdot\mathbf{C} - \mathbf{C}\cdot(\nabla\mathbf{u})^t + \frac{1}{\lambda_1}\mathbf{C}\right) : \mathbf{s}\,\mathrm{d}\mathbf{x} = \frac{1}{\lambda_1}\int_{\Omega\setminus\overline{B(t)}} \mathbf{I} : \mathbf{s}\,\mathrm{d}\mathbf{x}, \\ \forall\mathbf{s}\in\mathbf{W}, \end{cases} \tag{3.2.17}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{3.2.18}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega\setminus\overline{B(0)}, \tag{3.2.19}$$

$$\mathbf{C}(\mathbf{x},0) = \mathbf{C}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega, \tag{3.2.20}$$

$$\mathbf{G}(\mathbf{x},0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x},0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x},0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{3.2.21}$$

To obtain an equivalent fictitious domain formulation, first we fill B with a fluid of density ρ_f and suppose that this fluid follows the same rigid body motion as B itself, which is

$$\mathbf{u}(\mathbf{x},t) = \mathbf{V}(t) + \boldsymbol{\omega}(t)\times\overrightarrow{\mathbf{G}(t)\mathbf{x}}, \quad \forall\mathbf{x}\in B(t). \tag{3.2.22}$$

Define a function space

$$\widetilde{\mathbf{W}}_0(t) = \left\{ (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \,\middle|\, (\mathbf{v}|_{\Omega \setminus \overline{B(t)}}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{W}_0(t), \mathbf{v}(\mathbf{x}, t) = \mathbf{Y} + \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}(t)\mathbf{x}} \quad \forall \mathbf{x} \in B(t) \right\}.$$

Suppose particle B is made of an homogeneous material of density ρ_f which follows

$$\rho_f \int_{B(t)} \mathbf{g} \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} = \frac{\rho_f}{\rho_s} M_p \mathbf{g} \cdot \mathbf{Y}, \quad \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \widetilde{\mathbf{W}}_0(t), \tag{3.2.23}$$

$$\nabla \cdot \mathbf{v} = 0 \text{ in } B(t), \quad \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \widetilde{\mathbf{W}}_0(t), \tag{3.2.24}$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } B(t) \text{ and } \mathbf{D}(\mathbf{u}) = 0 \text{ in } B(t). \tag{3.2.25}$$

To obtain a fictitious domain formulation, we define the following function spaces

$$\mathbf{V}_{\mathbf{g}_0}(t) = \left\{ \mathbf{v} \,\middle|\, \mathbf{v} \in (H^1(\Omega))^3, \mathbf{v} = \mathbf{g}_0(t) \text{ on } \Gamma \right\},$$

$$L_0^2(\Omega) = \left\{ q \,\middle|\, q \in L^2(\Omega), \int_\Omega q \, \mathrm{d}\mathbf{x} = 0 \right\},$$

and

$$\mathbf{V}_{\mathbf{C}_L}(\Omega) = \left\{ \mathbf{A} \,\middle|\, \mathbf{A} \in \mathbf{W}(\Omega), \mathbf{A} = \mathbf{C}_L(t) \text{ on } \Gamma^- \right\},$$

$$\mathbf{V}_{\mathbf{C}_0}(\Omega) = \left\{ \mathbf{A} \,\middle|\, \mathbf{A} \in \mathbf{W}(\Omega), \mathbf{A} = 0 \text{ on } \Gamma^- \right\}.$$

Combining (3.2.15)-(3.2.21) with (3.2.22)-(3.2.25), we obtain the fictitious domain formulation as follows:

For a.e. $t \in (0, T)$, find $\mathbf{u}(t) \in \mathbf{V}_{\mathbf{g}_0}(t)$, $p(t) \in L_0^2(\Omega)$, $\mathbf{C}(t) \in \mathbf{V}_{\mathbf{C}_L}, \mathbf{V}(t) \in \mathbb{R}^3$,

$\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, such that ($p = 0$, $\mathbf{D}(\mathbf{u}) = 0$, $\mathbf{C} = I$, $\nabla \cdot \mathbf{u} = 0$ in B(t))

$$\begin{cases} -\displaystyle\int_\Omega p\nabla\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\,\mathrm{d}\mathbf{x} \\ -\dfrac{\eta}{\lambda_1}\displaystyle\int_\Omega \mathbf{v}\cdot(\nabla\cdot(\mathbf{C}-\mathbf{I}))\,\mathrm{d}\mathbf{x} + M_p\frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t}\cdot\mathbf{Y} + \frac{\mathrm{d}\left(\mathbf{I_p}\boldsymbol{\omega}\right)}{\mathrm{d}t}\cdot\boldsymbol{\theta} \\ -\mathbf{F}^r\cdot\mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r}\times\mathbf{F}^r\cdot\boldsymbol{\theta} = \rho_f\displaystyle\int_\Omega \mathbf{g}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + \left(1-\frac{\rho_f}{\rho_s}\right)M_p\mathbf{g}\cdot\mathbf{Y}, \\ \quad \forall(\mathbf{v},\mathbf{Y},\boldsymbol{\theta}) \in \widetilde{\mathbf{W}}_0(t), \end{cases} \tag{3.2.26}$$

$$\int_\Omega q\nabla\cdot\mathbf{u}\,\mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2(\Omega), \tag{3.2.27}$$

$$\begin{cases} \displaystyle\int_\Omega \left(\frac{\partial\mathbf{C}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{C} - (\nabla\mathbf{u})\cdot\mathbf{C} - \mathbf{C}\cdot(\nabla\mathbf{u})^t + \frac{1}{\lambda_1}\mathbf{C}\right) : \mathbf{s}\,\mathrm{d}\mathbf{x} = \frac{1}{\lambda_1}\int_\Omega \mathbf{I} : \mathbf{s}\,\mathrm{d}\mathbf{x}, \\ \quad \forall\mathbf{s} \in \mathbf{V}_{\mathbf{C}_0}, \mathbf{C} = \mathbf{I}\,\mathrm{in}\,B(t), \end{cases} \tag{3.2.28}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{3.2.29}$$

$$\mathbf{u}(\mathbf{x},t) = \mathbf{V}(t) + \boldsymbol{\omega}(t)\times\overrightarrow{\mathbf{G}(t)\mathbf{x}}, \quad \forall\mathbf{x}\in B(t). \tag{3.2.30}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega\setminus\overline{B(0)}, \tag{3.2.31}$$

$$\mathbf{C}(\mathbf{x},0) = \mathbf{C}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega, \tag{3.2.32}$$

$$\mathbf{G}(\mathbf{x},0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x},0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x},0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{3.2.33}$$

To relax the rigid body motion condition (3.2.30), we introduce a Lagrange multiplier, $\boldsymbol{\lambda} \in \Lambda(t) = (H^1(B(t)))^3$, and for any $\boldsymbol{\mu} \in (H^1(B(t)))^3$ and $\mathbf{v} \in (H^1(\Omega))^3$

such that

$$\langle \boldsymbol{\mu}, \mathbf{v} \rangle_{\Lambda(t)} = \int_{B(t)} \left(\boldsymbol{\mu} \cdot \mathbf{v} + \frac{1}{d^2} \nabla \boldsymbol{\mu} : \nabla \mathbf{v} \right) \mathrm{d}\mathbf{x},$$

where d is a scaling constant and, typically, has been used as the diameter of the particles.

Then we obtain the fictitious domain formulation over the entire region Ω as follows:

For a.e. $t \in (0, T)$, find $\mathbf{u}(t) \in \mathbf{V}_{\mathbf{g}_0}(t)$, $p(t) \in L_0^2(\Omega)$, $\mathbf{C}(t) \in \mathbf{V}_{\mathbf{C}_L}, \mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, $\boldsymbol{\lambda}(t) \in \Lambda(t)$ such that

$$\begin{cases} -\displaystyle\int_\Omega p \nabla \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + 2\mu_f \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v}) \, \mathrm{d}\mathbf{x} - \frac{\eta}{\lambda_1} \int_\Omega \mathbf{v} \cdot (\nabla \cdot (\mathbf{C} - \mathbf{I})) \, \mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} \cdot \mathbf{Y} + \dfrac{\mathrm{d}\left(\mathbf{I_p} \boldsymbol{\omega}\right)}{\mathrm{d}t} \cdot \boldsymbol{\theta} - \mathbf{F}^r \cdot \mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r} \times \mathbf{F}^r \cdot \boldsymbol{\theta} \\ -\left\langle \boldsymbol{\lambda}, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}\mathbf{x}} \right\rangle_{\Lambda(t)} = \rho_f \displaystyle\int_\Omega \mathbf{g} \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + \left(1 - \frac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y}, \\ \quad \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in (H_0^1(\Omega))^3 \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{3.2.34}$$

$$\int_\Omega q \nabla \cdot \mathbf{u} \, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2(\Omega), \tag{3.2.35}$$

$$\begin{cases} \displaystyle\int_\Omega \left(\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} - (\nabla \mathbf{u}) \cdot \mathbf{C} - \mathbf{C} \cdot (\nabla \mathbf{u})^t + \frac{1}{\lambda_1} \mathbf{C} \right) : \mathbf{s} \, \mathrm{d}\mathbf{x} = \frac{1}{\lambda_1} \int_\Omega \mathbf{I} : \mathbf{s} \, \mathrm{d}\mathbf{x}, \\ \quad \forall \mathbf{s} \in \mathbf{V}_{\mathbf{C}_0}, \mathbf{C} = \mathbf{I} \, \mathrm{in} \, B(t), \end{cases} \tag{3.2.36}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{3.2.37}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \overline{B(0)}, \tag{3.2.38}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u}(t) - \mathbf{V}(t) - \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G(t)x}} \right\rangle_{\Lambda(t)} = 0, \forall \boldsymbol{\mu} \in \Lambda(t), \tag{3.2.39}$$

$$\mathbf{C}(\mathbf{x}, 0) = \mathbf{C}_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \tag{3.2.40}$$

$$\mathbf{G}(\mathbf{x}, 0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x}, 0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x}, 0) = \boldsymbol{\omega}_0(\mathbf{x}). \tag{3.2.41}$$

Remark 3.2. *Since* $\mathbf{u}$ *is divergence free and satisfies the Dirichlet boundary conditions on* Γ, *we obtain*

$$2\int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\, d\mathbf{x} = \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\, d\mathbf{x}, \quad \forall \mathbf{v} \in (H_0^1(\Omega))^3.$$

So in relation (3.2.34) *we can replace* $2\int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\, d\mathbf{x}$ *by* $\int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\, d\mathbf{x}$. *Also the gravity* $\mathbf{g}$ *in* (3.2.34) *can be absorbed into the presure term.*

3.3 Numerical methods

3.3.1 Finite element approximation

For the purpose of finding an approximation solution of problem (3.2.34)-(3.2.41), we need a partition of the flow region $\Omega \in \mathbb{R}^3$. We use an uniform finite element mesh for Ω and let h be the uniform finite element mesh size for the velocity field, $\mathcal{T}_h$ be a tetrahedrization of Ω, and $\mathcal{T}_{2h}$ be twice coarser than $\mathcal{T}_h$.

For the space discretization, let P_i be the space of the polynomials in three variables of degree $\leq i$, we have chosen P_1-*iso*-P_2 finite element space for the velocity field and conformation tensor and P_1 finite elementspace for the pressure. Then we have the following function spaces:

$$\mathbf{V}_h = \left\{ \mathbf{v}_h \middle| \mathbf{v}_h \in \left(C^0(\bar{\Omega})\right)^3, \mathbf{v}_h\,|_T \in (P_1)^3, \forall T \in \mathcal{T}_h \right\},$$

$$\mathbf{V}_{\mathbf{g}_{0h}(t)} = \{ \mathbf{v}_h \,|\mathbf{v}_h \in \mathbf{V}_h, \mathbf{v}_h\,|_\Gamma = \mathbf{g}_{0h}(t) \},$$

$$\mathbf{V}_{0h} = \{ \mathbf{v}_h \,|\mathbf{v}_h \in \mathbf{V}_h, \mathbf{v}_h\,|_\Gamma = 0 \},$$

$$L_h^2 = \left\{ q_h \,\middle| q_h \in C^0(\bar{\Omega}), q_h\,|_T \in P_1, \forall T \in \mathcal{T}_{2h} \right\},$$

$$L_{0h}^2 = \left\{ q_h \middle| q_h \in L_h^2, \int_\Omega q_h \, \mathrm{d}\mathbf{x} = 0 \right\},$$

$$\mathbf{V}_{\mathbf{C}_{L_h}} = \left\{ \mathbf{s}_h \middle| \mathbf{s}_h \in \left(C^0(\bar{\Omega})\right)^{3\times 3}, \mathbf{s}_h \middle|_T \in (P_1)^{3\times 3}, \forall T \in \mathcal{T}_h, \mathbf{s}_h \middle|_{\Gamma_h^-} = \mathbf{C}_{L_h(t)} \right\},$$

and

$$\mathbf{V}_{\mathbf{C}_{0h}} = \left\{ \mathbf{s}_h \middle| \mathbf{s}_h \in \left(C^0(\bar{\Omega})\right)^{3\times 3}, \mathbf{s}_h \middle|_T \in (P_1)^{3\times 3}, \forall T \in \mathcal{T}_h, \mathbf{s}_h \middle|_{\Gamma_h^-} = 0 \right\},$$

where $\mathbf{g}_{0h}(t)$ is an approximation of $\mathbf{g}_0(t)$ satisfying

$$\int_\Gamma \mathbf{g}_{0h}(t) \cdot \mathbf{n} \mathrm{d}\Gamma = 0,$$

and

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

For simulating the particle motion in fluid flow, we need to define a finite dimensional space to approach the space of Lagrange multipier $\Lambda(t)$. Let $\{\boldsymbol{\xi}_i\}_{i=1}^{N(t)}$ be a set of points from $\overline{B(t)}$ which cover $\overline{B(t)}$ evenly. We define the discrete Lagrange multiplier space by

$$\Lambda_h(t) = \left\{ \boldsymbol{\mu}_h \;\middle|\; \boldsymbol{\mu}_h = \sum_{i=1}^{N(t)} \boldsymbol{\mu}_i \delta(\mathbf{x} - \boldsymbol{\xi}_i), \boldsymbol{\mu}_i \in \mathbb{R}^3, \forall i = 1, \cdots, N(t) \right\},$$

where $\mathbf{x} \to \delta(\mathbf{x} - \boldsymbol{\xi}_i)$ is the Dirac measure at $\mathbf{x} = \boldsymbol{\xi}_i$. Then we define a pairing over $\Lambda_h(t) \times \mathbf{V}_{\mathbf{g}_{0h}(t)}$ (or $\Lambda_h(t) \times \mathbf{V}_{\mathbf{g}_0}$) by

$$\langle \boldsymbol{\mu}_h, \mathbf{v}_h \rangle_{\Lambda_h(t)} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \cdot \mathbf{v}_h(\boldsymbol{\xi}_i), \tag{3.3.42}$$

for $\boldsymbol{\mu}_h \in \boldsymbol{\Lambda}_h(t), \mathbf{v}_h \in \mathbf{V}_{\mathbf{g}_{0h}(t)}$ or $\mathbf{V}_{0h}$. A typical set $\{\boldsymbol{\xi}_i\}_{i=1}^{N(t)}$ of points from $\overline{B(t)}$ to be used in (3.3.42) is defined as

$$\{\boldsymbol{\xi}_i\}_{i=1}^{N(t)} = \{\boldsymbol{\xi}_i\}_{i=1}^{N_1(t)} \bigcup \{\boldsymbol{\xi}_i\}_{i=N_1(t)+1}^{N(t)},$$

where $\{\boldsymbol{\xi}_i\}_{i=1}^{N_1(t)}$ is the set of those vertices of the velocity grid $\mathcal{T}_h$ contained in $B(t)$ and the distance between those vertices and the boundary $\partial B(t)$ is greater than or equal to $\frac{h}{2}$, and selected points $\{\boldsymbol{\xi}_i\}_{i=N_1(t)+1}^{N(t)}$ from $\partial B(t)$. For simulating particle interactions in Stokes flow, we define a modified pairing $< \cdot, \cdot >_{\Lambda_h(t)}$ as follows:

$$\langle \boldsymbol{\mu}_h, \mathbf{v}_h \rangle_{\Lambda_h(t)} = \sum_{i=1}^{N_1(t)} \boldsymbol{\mu}_i \cdot \mathbf{v}_h(\boldsymbol{\xi}_i) + \sum_{i=N_1(t)+1}^{N(t)} \sum_{j=1}^{M} \boldsymbol{\mu}_i \cdot \mathbf{v}_h(\boldsymbol{\xi}_i) D_h(\boldsymbol{\xi}_i - \mathbf{x}_j) h^3, \tag{3.3.43}$$

for $\boldsymbol{\mu}_h \in \Lambda_h(t), \mathbf{v}_h \in \mathbf{V}_{\mathbf{g}_{0h}(t)}$ or $\mathbf{V}_{0h}$ where $\{\mathbf{x}_j\}_{j=1}^{M}$ are the grid points of the finite elements for the velocity, and the function $D_h(\mathbf{X} - \boldsymbol{\xi}_i)$ is defined as

$$D_h(\mathbf{X} - \boldsymbol{\xi}_i) = \delta_h(X_1 - \xi_{i1}) \delta_h(X_2 - \xi_{i2}) \delta_h(X_3 - \xi_{i3}),$$

with $\mathbf{X} = (X_1, X_2, X_3)^t$ and $\xi_i = (\xi_{i1}, \xi_{i2}, \xi_{i3})^t$, and the one-dimensional approximate Dirac measure δ_h being defined by

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

By using the above pairing $< \cdot, \cdot >_{\Lambda_h(t)}$, the rigid body motion of particle $B(t)$ is forced via an immersed boundary method develped by Peskin.

Based on the finite dimensional spaces above, we obtain the following approximation of problem (3.2.34)- (3.2.41) :

For a.e. $t \in (0, T)$, find $\mathbf{u}_h(t) \in \mathbf{V}_{\mathbf{g}_{0h}}(t)$, $p(t) \in L^2_{0h}$, $\mathbf{C}_h(t) \in \mathbf{V}_{\mathbf{C}_{L_h}(t)}$,$\mathbf{V}(t) \in \mathbb{R}^3$, $\mathbf{G}(t) \in \mathbb{R}^3$, $\boldsymbol{\omega}(t) \in \mathbb{R}^3$, $\boldsymbol{\lambda}_h \in \Lambda_h(t)$ such that

$$\begin{cases} -\displaystyle\int_\Omega p \nabla \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + \mu_f \int_\Omega \nabla \mathbf{u}_h : \nabla \mathbf{v} \, \mathrm{d}\mathbf{x} - \frac{\eta}{\lambda_1} \int_\Omega \mathbf{v} \cdot (\nabla \cdot (\mathbf{C}_h - \mathbf{I})) \, \mathrm{d}\mathbf{x} + M_p \frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} \cdot \mathbf{Y} + \frac{\mathrm{d}\,(\mathbf{I_p}\boldsymbol{\omega})}{\mathrm{d}t} \cdot \boldsymbol{\theta} \\ -\mathbf{F}^r \cdot \mathbf{Y} - \overrightarrow{\mathbf{G}\mathbf{x}_r} \times \mathbf{F}^r \cdot \boldsymbol{\theta} = \left(1 - \dfrac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} + \left\langle \boldsymbol{\lambda}_h, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}\mathbf{x}} \right\rangle_{\Lambda_h(t)}, \\ \quad \forall (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{V}_{0h} \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{3.3.44}$$

$$\int_\Omega q \nabla \cdot \mathbf{u}_h \, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2_h, \tag{3.3.45}$$

$$\begin{cases} \displaystyle\int_\Omega \left(\frac{\partial \mathbf{C}_h}{\partial t} + (\mathbf{u}_h \cdot \nabla)\mathbf{C}_h - (\nabla \mathbf{u}_h) \cdot \mathbf{C}_h - \mathbf{C}_h \cdot (\nabla \mathbf{u}_h)^t + \frac{1}{\lambda_1}\mathbf{C}_h \right) : \mathbf{s}_h \, \mathrm{d}\mathbf{x} = \frac{1}{\lambda_1} \int_\Omega \mathbf{I} : \mathbf{s}_h \, \mathrm{d}\mathbf{x}, \\ \qquad \forall \mathbf{s}_h \in \mathbf{V}_{\mathbf{C}_{0h}}, \mathbf{C}_h = \mathbf{I} \text{ in } B_h(t), \end{cases} \tag{3.3.46}$$

$$\frac{\mathrm{d}\mathbf{G}}{\mathrm{d}t} = \mathbf{V}, \tag{3.3.47}$$

$$\mathbf{u}_h(\mathbf{x}, 0) = \mathbf{u}_{0h}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \overline{B_h(0)}, \tag{3.3.48}$$

$$\left\langle \boldsymbol{\mu}_h, \mathbf{u}_h(t) - \mathbf{V}(t) - \boldsymbol{\omega}(t) \times \overrightarrow{\mathbf{G(t)x}} \right\rangle_{\Lambda_h(t)} = 0, \forall \mu_h \in \Lambda_h(t), \tag{3.3.49}$$

$$\mathbf{C}_h(\mathbf{x}, 0) = \mathbf{C}_{0h}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \tag{3.3.50}$$

$$\mathbf{G}(\mathbf{x}, 0) = \mathbf{G}_0(\mathbf{x}), \quad \mathbf{V}(\mathbf{x}, 0) = \mathbf{V}_0(\mathbf{x}), \quad \boldsymbol{\omega}(\mathbf{x}, 0) = \boldsymbol{\omega}_0(\mathbf{x}), \tag{3.3.51}$$

where $\mathbf{u}_{0h}$ is an approximation of $\mathbf{u}_0$ such that

$$\int_\Omega q \nabla \cdot \mathbf{u}_{0h} \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2_h.$$

Remark 3.3. *If we consider our particle as a sphere, the moment of inertia* $\mathbf{I}_p$ *is a constant with respect to time* t*. Then in relation* (3.3.44) *the term* $\dfrac{d\left(\mathbf{I_p}\boldsymbol{\omega}\right)}{dt}$ *can be rewriten as* $\mathbf{I_p}\dfrac{d\boldsymbol{\omega}}{dt}$*.*

3.3.2 Operator splitting scheme

Consider the following initial value problem:

$$\begin{cases} \dfrac{\mathrm{d}\phi}{\mathrm{d}t} + A(\phi) = 0 \text{ on } (0, T), \\ \phi(0) = \phi_0, \end{cases}$$

with $0 < T < +\infty$. We suppose that operator A has a decompsition such as $A = \sum_{j=1}^{J} A_j$ with $J \geq 2$.

Let $\tau > 0$ be a time-discretization step, we denote $n\tau$ by t^n. By setting ϕ^n as an approximation of $\phi(t^n)$, we can write down the Lie's scheme as follows: Given $\phi^0 = \phi_0$. For $n \geq 0$, ϕ^n is known and we compute ϕ^{n+1} via

$$\begin{cases} \dfrac{\mathrm{d}\phi}{\mathrm{d}t} + A_j(\phi) = 0 \text{ on } (t^n, t^{n+1}), \\ \phi(t^n) = \phi^{n+\frac{j-1}{J}}; \phi^{n+\frac{j}{J}} = \phi(t^{n+1}), \end{cases}$$

for $j = 1, \cdots, J$.

Since the conformation tensor $\mathbf{C}$ is symmetric and positive definite, by Cholesky factorization there is a 3×3 lower triangular matrix $\mathbf{A}$ such that $\mathbf{C} = \mathbf{A}\mathbf{A}^t$, where $\mathbf{A}^t$ is the transpose matrix of $\mathbf{A}$. To split the constitutive equation with respect to $\mathbf{C}$, we have derived the following results.

Lemma 3.4. *For a lower triangular matrix $\mathbf{A}$ and $\mathbf{C} = \mathbf{A}\mathbf{A}^t$, given $\mathbf{u} \in \mathbb{R}^3$ and a positvie constant λ_1, we have*

(i) if $\mathbf{A}$ satisfies the equation $\dfrac{d\mathbf{A}}{dt} + (\mathbf{u} \cdot \nabla)\mathbf{A} = 0$, then $\mathbf{C}$ satisfies the equation $\dfrac{d\mathbf{C}}{dt} + (\mathbf{u} \cdot \nabla)\mathbf{C} = 0$;

(ii) if $\mathbf{A}$ satisfies the equation $\dfrac{d\mathbf{A}}{dt} + \dfrac{1}{2\lambda_1}\mathbf{A} - (\nabla\mathbf{u})\mathbf{A} = 0$, then $\mathbf{C}$ satisfies the equation
$\dfrac{d\mathbf{C}}{dt} + \dfrac{1}{\lambda_1}\mathbf{C} - (\nabla\mathbf{u})\mathbf{C} - \mathbf{C}(\nabla\mathbf{u})^t = 0.$

Proof. (i) Given $\dfrac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} + (\mathbf{u} \cdot \nabla)\mathbf{A} = 0$. Mulitplying the equation by $\mathbf{A}^t$ to the right, we obtain

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}\mathbf{A}^t + (\mathbf{u}\cdot\nabla)\mathbf{A}\mathbf{A}^t = 0. \tag{3.3.52}$$

Mulitplying the transpose of the equation by $\mathbf{A}$ to the left, we obtain

$$\mathbf{A}\frac{\mathrm{d}\mathbf{A}^t}{\mathrm{d}t} + \mathbf{A}(\mathbf{u}\cdot\nabla)\mathbf{A}^t = 0. \tag{3.3.53}$$

Adding (3.3.52) and (3.3.53) gives

$$\frac{\mathrm{d}\left(\mathbf{A}\mathbf{A}^t\right)}{\mathrm{d}t} + (\mathbf{u}\cdot\nabla)\left(\mathbf{A}\mathbf{A}^t\right) = 0.$$

Thus, we get

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} + (\mathbf{u}\cdot\nabla)\mathbf{C} = 0.$$

(ii) Given $\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} + \frac{1}{2\lambda_1}\mathbf{A} - (\nabla\mathbf{u})\mathbf{A} = 0$. Mulitplying the equation by $\mathbf{A}^t$ to the right, we obtain

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}\mathbf{A}^t + \frac{1}{2\lambda_1}\mathbf{A}\mathbf{A}^t - (\nabla\mathbf{u})\mathbf{A}\mathbf{A}^t = 0 \tag{3.3.54}$$

Mulitplying the transpose of the equation by $\mathbf{A}$ to the left, we obtain

$$\mathbf{A}\frac{\mathrm{d}\mathbf{A}^t}{\mathrm{d}t} + \frac{1}{2\lambda_1}\mathbf{A}\mathbf{A}^t - \mathbf{A}\mathbf{A}^t(\nabla\mathbf{u})^t = 0 \tag{3.3.55}$$

Adding (3.3.54) and (3.3.55) gives

$$\frac{\mathrm{d}\left(\mathbf{A}\mathbf{A}^t\right)}{\mathrm{d}t} + \frac{1}{\lambda_1}\mathbf{A}\mathbf{A}^t - (\nabla\mathbf{u})\mathbf{A}\mathbf{A}^t - \mathbf{A}\mathbf{A}^t(\nabla\mathbf{u})^t = 0.$$

Thus, we get

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} + \frac{1}{\lambda_1}\mathbf{C} - (\nabla\mathbf{u})\mathbf{C} - \mathbf{C}(\nabla\mathbf{u})^t = 0.$$

□

Similarly, we can define finite dimensional spaces $\mathbf{V}_{\mathbf{A}_{L_h}(t)}$ or $\mathbf{V}_{\mathbf{A}_{0h}}$ for $\mathbf{A}$.

Applying the Lie's scheme to the discrete analogue of the problem (3.3.44)-(3.3.51) with $\mathbf{C} = \mathbf{A}\mathbf{A}^t$ and the backward Euler's method to some subproblems, we obtain:

Given $\mathbf{u}^0 = \mathbf{u}_{0h}, \mathbf{C}^0 = \mathbf{C}_{0h}, \mathbf{G}^0 = \mathbf{G}_0, \mathbf{V}^0 = \mathbf{V}_0, \boldsymbol{\omega}^0 = \boldsymbol{\omega}_0$. For $n \geq 0$, $\mathbf{u}^n, \mathbf{C}^n, \mathbf{G}^n, \mathbf{V}^n, \boldsymbol{\omega}^n$ are known, we first predict the position and the translation velocity of the center of mass as follows.

$$\frac{d\mathbf{G}}{dt} = \mathbf{V}(t), \tag{3.3.56}$$

$$M_p\frac{d\mathbf{V}}{dt} = \mathbf{0}, \tag{3.3.57}$$

$$\mathbf{I_p}\frac{d\boldsymbol{\omega}}{dt} = \mathbf{0}, \tag{3.3.58}$$

$$\mathbf{V}(t^n) = \mathbf{V}^n, \boldsymbol{\omega}(t^n) = \boldsymbol{\omega}^n, \mathbf{G}(t^n) = \mathbf{G}^n, \tag{3.3.59}$$

for $t^n < t < t^{n+1}$. Then set $\mathbf{V}^{n+\frac{1}{4}} = \mathbf{V}(t^{n+1})$, $\boldsymbol{\omega}^{n+\frac{1}{4}} = \boldsymbol{\omega}(t^{n+1})$, and $\mathbf{G}^{n+\frac{1}{4}} = \mathbf{G}(t^{n+1})$. With the center $\mathbf{G}^{n+1}$ we get in the above step, the region of B_h^{n+1} occupied by the particle is determined and we set $\mathbf{C}^{n+\frac{1}{4}} = \mathbf{I}$ in B_h^{n+1} and $\mathbf{C}^{n+\frac{1}{4}} = \mathbf{C}^n$ otherwise.

Then we enforce the rigid body motion in B_h^{n+1} and solve $\mathbf{u}^{n+1}$ and p^{n+1} simultaneously as follows:

Find $\mathbf{u}^{n+1} \in \mathbf{V}_{\mathbf{g}_{0h}}^{n+1}$, $p^{n+1} \in L_{0h}^2$, $\boldsymbol{\lambda}^{n+1} \in \Lambda_h^{n+1}$, $\mathbf{V}^{n+1} \in \mathbb{R}^3$, $\boldsymbol{\omega}^{n+1} \in \mathbb{R}^3$ such that

$$\begin{cases} -\displaystyle\int_\Omega p^{n+1} \nabla \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} + \mu_f \int_\Omega \nabla \mathbf{u}^{n+1} : \nabla \mathbf{v} \, \mathrm{d}\mathbf{x} - \frac{\eta}{\lambda_1} \int_\Omega \mathbf{v} \cdot \left(\nabla \cdot \left(\mathbf{C}^{n+\frac{1}{4}} - \mathbf{I}\right)\right) \mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathbf{V}^{n+1} - \mathbf{V}^{n+\frac{1}{4}}}{\triangle t} \cdot \mathbf{Y} + \mathbf{I_p} \dfrac{\boldsymbol{\omega}^{n+1} - \boldsymbol{\omega}^{n+\frac{1}{4}}}{\Delta t} \cdot \boldsymbol{\theta} \\ = \left(1 - \dfrac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} + \left\langle \boldsymbol{\lambda}^{n+1}, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{G}^{n+1}\mathbf{x}} \right\rangle_{\Lambda_h^{n+1}}, \\ \quad \forall \; (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{V}_{0h} \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{3.3.60}$$

$$\int_\Omega q \nabla \cdot \mathbf{u}^{n+1} \, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L_h^2, \tag{3.3.61}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u}^{n+1} - \mathbf{V}^{n+1} - \boldsymbol{\omega}^{n+1} \times \overrightarrow{\mathbf{G}^{n+1}\mathbf{x}} \right\rangle_{\Lambda_h^{n+1}} = 0, \quad \forall \boldsymbol{\mu} \in \Lambda_h^{n+1}. \tag{3.3.62}$$

and set $\mathbf{C}^{n+\frac{2}{4}} = \mathbf{C}^{n+\frac{1}{4}}$.

Next, we set $\mathbf{A}^{n+\frac{2}{4}}(\mathbf{A}^{n+\frac{2}{4}})^t = \mathbf{C}^{n+\frac{2}{4}}$ and compute $\mathbf{A}^{n+\frac{3}{4}}$ via the solution of

$$\begin{cases} \displaystyle\int_\Omega \frac{\mathrm{d}\mathbf{A}(t)}{\mathrm{d}t} : \mathbf{s} \, \mathrm{d}\mathbf{x} + \int_\Omega \left(\mathbf{u}^n \cdot \nabla\right) \mathbf{A}(t) : \mathbf{s} \, \mathrm{d}\mathbf{x} = 0, \forall \mathbf{s} \in \mathbf{V}_{\mathbf{A}_{0h}} \\ \mathbf{A}(t^n) = \mathbf{A}^{n+\frac{2}{4}}, \\ \mathbf{A}(t) \in \mathbf{V}_{\mathbf{A}_{L_h}}^{n+1}, t \in [t^n, t^{n+1}] \end{cases} \tag{3.3.63}$$

and set $\mathbf{A}(t^{n+1}) = \mathbf{A}^{n+\frac{3}{4}}$ and $\mathbf{u}^{n+\frac{3}{4}} = \mathbf{u}^{n+\frac{2}{4}}$.

Then we compute $\mathbf{A}^{n+1}$ via the solution of

$$\begin{cases} \displaystyle\int_\Omega \left[\frac{\mathbf{A}^{n+1} - \mathbf{A}^{n+\frac{3}{4}}}{\Delta t} - \left(\nabla \mathbf{u}^n\right) \mathbf{A}^{n+1} + \frac{1}{2\lambda_1} \mathbf{A}^{n+1}\right] : \mathbf{s} \, \mathrm{d}\mathbf{x} = 0, \\ \forall \mathbf{s} \in \mathbf{V}_{\mathbf{A}_{0h}}, \mathbf{A}^{n+1} \in \mathbf{V}_{\mathbf{A}_{L_h}}^{n+1}, \end{cases} \tag{3.3.64}$$

and set

$$\mathbf{C}^{n+1} = \mathbf{A}^{n+1}(\mathbf{A}^{n+1})^t + \frac{1}{\lambda_1}\mathbf{I}. \tag{3.3.65}$$

In the above, $\mathbf{V}^{n+1}_{\mathbf{A}_{L_h}} = \mathbf{V}_{\mathbf{A}_{L_h}(t^{n+1})}$, $\mathbf{V}^{n+1}_{\mathbf{g}_{0h}} = \mathbf{V}_{\mathbf{g}_{0h}(t^{n+1})}$, $\Lambda^{n+1}_h = \Lambda_h(t^{n+1})$, and $B^{n+s}_h = B_h(t^{n+s})$ where the spaces $\mathbf{V}_{\mathbf{A}_{L_h}(t)}$ and $\mathbf{V}_{\mathbf{A}_{0h}}$ for $\mathbf{A}$ are defined similar to those $\mathbf{V}_{\mathbf{C}_{L_h}(t)}$ and $\mathbf{V}_{\mathbf{C}_{0h}}$.

3.3.3 Logarithm of conformation tensor

Besides matrix factorization approach, we consider the log-conformation representation for the conformation tensor.

add the derivation of logarithm conformation.

In order to resolve the exponential behavior of the conformation tensor, we replace (3.3.63) – (3.3.65) by (3.3.66) – (3.3.68) when solving the constitutive equation:

We set $\boldsymbol{\psi}^{n+\frac{2}{4}} = log\left(\mathbf{C}^{n+\frac{2}{4}}\right)$ and compute $\boldsymbol{\psi}^{n+\frac{3}{4}}$ via the solution of

$$\begin{cases} \int_\Omega \frac{\partial \boldsymbol{\psi}(t)}{\partial t} : \mathbf{s}\,d\mathbf{x} + \int_\Omega (\mathbf{u}^n \cdot \nabla)\,\boldsymbol{\psi}(t) : \mathbf{s}\,d\mathbf{x} = 0, \forall \mathbf{s} \in \mathbf{V}_{\mathbf{C}_{0h}} \\ \boldsymbol{\psi}(t^n) = \boldsymbol{\psi}^{n+\frac{2}{4}}, \\ \boldsymbol{\psi}(t) \in \mathbf{V}^{n+1}_{\mathbf{C}_{L_h}}, t \in [t^n, t^{n+1}] \end{cases} \tag{3.3.66}$$

and set $\boldsymbol{\psi}^{n+\frac{3}{4}} = \boldsymbol{\psi}(t^{n+1})$ and $\mathbf{u}^{n+\frac{3}{4}} = \mathbf{u}^{n+\frac{2}{4}}$.

Then, we set $\mathbf{C}^{n+\frac{3}{4}} = e^{\boldsymbol{\psi}^{n+\frac{3}{4}}}$ and $\mathbf{O}^{n+\frac{3}{4}} + \mathbf{S}^{n+\frac{3}{4}} + \mathbf{N}^{n+\frac{3}{4}}\left(\mathbf{C}^{n+\frac{3}{4}}\right)^{-1} = \nabla \mathbf{u}^{n+\frac{3}{4}}$ and compute $\boldsymbol{\psi}^{n+1}$ via the solution of

$$\begin{cases} \dfrac{\partial \boldsymbol{\psi}(t)}{\partial t} - \left(\mathbf{O}^{n+\frac{3}{4}}\boldsymbol{\psi}(t) - \boldsymbol{\psi}(t)\mathbf{O}^{n+\frac{3}{4}}\right) - 2\mathbf{S}^{n+\frac{3}{4}} = 0, \\ \boldsymbol{\psi}(t^n) = \boldsymbol{\psi}^{n+\frac{3}{4}}, \\ \boldsymbol{\psi}(t) \in \mathbf{V}^{n+1}_{\mathbf{C}_{L_h}}, t \in [t^n, t^{n+1}] \end{cases} \tag{3.3.67}$$

and set $\boldsymbol{\psi}^{n+1} = \boldsymbol{\psi}(t^{n+1})$ and $\mathbf{C}^{n+1} = e^{\boldsymbol{\psi}^{n+1}}$. Then solve the ODE

$$\begin{cases} \dfrac{\partial \mathbf{C}}{\partial t} = \dfrac{1}{\lambda_1}(\mathbf{I} - \mathbf{C}), \\ \mathbf{C}(t^n) = \mathbf{C}^{n+1}, \\ \mathbf{C}(t) \in \mathbf{V}^{n+1}_{\mathbf{C}_{L_h}}, t \in [t^n, t^{n+1}] \end{cases} \tag{3.3.68}$$

In (3.3.67), it is better to use exact solution instead of the approxiamtion from the first order scheme.

3.3.4 Operator splitting scheme of Carreau model

To consider the operator splitting scheme of Carreau model, we have:

Given $\mathbf{u}^0 = \mathbf{u}_{0h}, \mathbf{C}^0 = \mathbf{C}_{0h}, \mathbf{G}^0 = \mathbf{G}_0, \mathbf{V}^0 = \mathbf{V}_0, \boldsymbol{\omega}^0 = \boldsymbol{\omega}_0$. For $n \geq 0$, $\mathbf{u}^n, \mathbf{C}^n, \mathbf{G}^n, \mathbf{V}^n, \boldsymbol{\omega}^n$ are known, we first predict the position and the translation velocity of the center of mass as follows. Taking $\mathbf{V}^{n+\frac{1}{4},0} = \mathbf{V}^n$ and $\mathbf{G}^{n+1,0} = \mathbf{G}^n$, for $k = 1, 2, \cdots, N$, computing

$$\frac{d\mathbf{G}}{dt} = \mathbf{V}(t), \tag{3.3.69}$$

$$M_p \frac{d\mathbf{V}}{dt} = \mathbf{0}, \tag{3.3.70}$$

$$\mathbf{I_p} \frac{d\boldsymbol{\omega}}{dt} = \mathbf{0}, \tag{3.3.71}$$

$$\mathbf{V}(t^n) = \mathbf{V}^n, \boldsymbol{\omega}(t^n) = \boldsymbol{\omega}^n, \mathbf{G}(t^n) = \mathbf{G}^n, \tag{3.3.72}$$

for $t^n < t < t^{n+1}$.Then set $\mathbf{V}^{n+\frac{1}{4}} = \mathbf{V}(t^{n+1})$, $\boldsymbol{\omega}^{n+\frac{1}{4}} = \boldsymbol{\omega}(t^{n+1})$, and $\mathbf{G}^{n+\frac{1}{4}} = \mathbf{G}(t^{n+1})$. With the center $\mathbf{G}^{n+1}$ we get in the above step, the region of B_h^{n+1} occupied by the particle is determined and we set $\mathbf{C}^{n+\frac{1}{4}} = \mathbf{I}$ in B_h^{n+1} and $\mathbf{C}^{n+\frac{1}{4}} = \mathbf{C}^n$ otherwise.

Then we calculate $\eta_1(\dot{\gamma}^n)$ by using the previous time step velocity $\mathbf{u}^n$ and set $\mu(\dot{\gamma}^n) = \eta_1(\dot{\gamma}^n)\dfrac{\lambda_2}{\lambda_1}$ and $\eta(\dot{\gamma}^n) = \eta_1(\dot{\gamma}^n) - \mu(\dot{\gamma}^n)$, enforce the rigid body motion in B_h^{n+1} and solve $\mathbf{u}^{n+1}$ and p^{n+1} simultaneously as follows:

Find $\mathbf{u}^{n+1} \in \mathbf{V}_{\mathbf{g}_{0h}}^{n+1}$, $p^{n+1} \in L_{0h}^2$, $\boldsymbol{\lambda}^{n+1} \in \Lambda_h^{n+1}$, $\mathbf{V}^{n+1} \in \mathbb{R}^3$, $\boldsymbol{\omega}^{n+1} \in \mathbb{R}^3$ such that

$$\left(\dot{\gamma}^n\right)^2 = 2\mathbf{D}(\mathbf{u}^n) : \mathbf{D}(\mathbf{u}^n),$$

$$\eta_1\left(\dot{\gamma}^n\right) = \frac{\eta_1}{\left(1 + (\lambda_1 \dot{\gamma}^n)^2\right)^{\frac{1-n}{2}}}, \quad \mu\left(\dot{\gamma}^n\right) = \eta_1\left(\dot{\gamma}^n\right)\frac{\lambda_2}{\lambda_1}, \quad \eta\left(\dot{\gamma}^n\right) = \eta_1\left(\dot{\gamma}^n\right) - \mu\left(\dot{\gamma}^n\right),$$

$$\left\{\begin{array}{l} -\displaystyle\int_\Omega p^{n+1}\nabla\cdot\mathbf{v}\,\mathrm{d}\mathbf{x}+\mu_f\int_\Omega\nabla\mathbf{u}^{n+1}:\nabla\mathbf{v}\,\mathrm{d}\mathbf{x}+M_p\frac{\mathbf{V}^{n+1}-\mathbf{V}^{n+\frac{1}{4}}}{\triangle t}\cdot\mathbf{Y}+\mathbf{I_p}\frac{\boldsymbol{\omega}^{n+1}-\boldsymbol{\omega}^{n+\frac{1}{4}}}{\triangle t}\cdot\boldsymbol{\theta}\\ =2\displaystyle\int_\Omega\left(\mu_f-\mu\left(\dot{\gamma}^n\right)\right)\left(\mathbf{D}(\mathbf{u}^n):\nabla\mathbf{v}\right)\,\mathrm{d}\mathbf{x}+\int_\Omega\mathbf{v}\cdot\left(\nabla\cdot\frac{\eta\left(\dot{\gamma}^n\right)}{\lambda_1}\left(\mathbf{C}^{n+\frac{1}{4}}-\mathbf{I}\right)\right)\,\mathrm{d}\mathbf{x}\\ +\left(1-\dfrac{\rho_f}{\rho_s}\right)M_p\mathbf{g}\cdot\mathbf{Y}+\left\langle\boldsymbol{\lambda}^{n+1},\mathbf{v}-\mathbf{Y}-\boldsymbol{\theta}\times\overrightarrow{\mathbf{G}^{n+1}\mathbf{x}}\right\rangle_{\Lambda_h^{n+1}},\\ \quad\forall\,(\mathbf{v},\mathbf{Y},\boldsymbol{\theta})\in\mathbf{V}_{0h}\times\mathbb{R}^3\times\mathbb{R}^3, \end{array}\right. \tag{3.3.73}$$

$$\int_\Omega q\nabla\cdot\mathbf{u}^{n+1}\,\mathrm{d}\mathbf{x}=0,\quad\forall q\in L_h^2, \tag{3.3.74}$$

$$\left\langle\boldsymbol{\mu},\mathbf{u}^{n+1}-\mathbf{V}^{n+1}-\boldsymbol{\omega}^{n+1}\times\overrightarrow{\mathbf{G}^{n+1}\mathbf{x}}\right\rangle_{\Lambda_h^{n+1}}=0,\quad\forall\boldsymbol{\mu}\in\Lambda_h^{n+1}. \tag{3.3.75}$$

and set $\mathbf{C}^{n+\frac{2}{4}}=\mathbf{C}^{n+\frac{1}{4}}$.

Next, we set $\mathbf{A}^{n+\frac{2}{4}}(\mathbf{A}^{n+\frac{2}{4}})^t=\mathbf{C}^{n+\frac{2}{4}}$ and compute $\mathbf{A}^{n+\frac{3}{4}}$ via the solution of

$$\left\{\begin{array}{c} \displaystyle\int_\Omega\frac{\mathrm{d}\mathbf{A}(t)}{\mathrm{d}t}:\mathbf{s}\,\mathrm{d}\mathbf{x}+\int_\Omega\left(\mathbf{u}^n\cdot\nabla\right)\mathbf{A}(t):\mathbf{s}\,\mathrm{d}\mathbf{x}=0,\forall\mathbf{s}\in\mathbf{V}_{\mathbf{A}_{0h}}\\ \mathbf{A}(t^n)=\mathbf{A}^{n+\frac{2}{4}},\\ \mathbf{A}(t)\in\mathbf{V}^{n+1}_{\mathbf{A}_{L_h}},t\in[t^n,t^{n+1}] \end{array}\right. \tag{3.3.76}$$

and set $\mathbf{A}(t^{n+1})=\mathbf{A}^{n+\frac{3}{4}}$ and $\mathbf{u}^{n+\frac{3}{4}}=\mathbf{u}^{n+\frac{2}{4}}$.

Then we compute $\mathbf{A}^{n+1}$ via the solution of

$$\left\{\begin{array}{c} \displaystyle\int_\Omega\left[\frac{\mathbf{A}^{n+1}-\mathbf{A}^{n+\frac{3}{4}}}{\triangle t}-\left(\nabla\mathbf{u}^n\right)\mathbf{A}^{n+1}+\frac{1}{2\lambda_1}\mathbf{A}^{n+1}\right]:\mathbf{s}\,\mathrm{d}\mathbf{x}=0,\\ \forall\mathbf{s}\in\mathbf{V}_{\mathbf{A}_{0h}},\mathbf{A}^{n+1}\in\mathbf{V}^{n+1}_{\mathbf{A}_{L_h}}, \end{array}\right. \tag{3.3.77}$$

and set

$$\mathbf{C}^{n+1} = \mathbf{A}^{n+1}(\mathbf{A}^{n+1})^t + \frac{1}{\lambda_1}\mathbf{I}. \tag{3.3.78}$$

In the above,$\mathbf{V}^{n+1}_{\mathbf{A}_{L_h}} = \mathbf{V}_{\mathbf{A}_{L_h}(t^{n+1})}$, $\mathbf{V}^{n+1}_{\mathbf{g}_{0h}} = \mathbf{V}_{\mathbf{g}_{0h}(t^{n+1})}$, $\Lambda^{n+1}_h = \Lambda_h(t^{n+1})$, and $B^{n+s}_h = B_h(t^{n+s})$ where the spaces $\mathbf{V}_{\mathbf{A}_{L_h}(t)}$ and $\mathbf{V}_{\mathbf{A}_{0h}}$ for $\mathbf{A}$ are defined similar to those $\mathbf{V}_{\mathbf{C}_{L_h}(t)}$ and $\mathbf{V}_{\mathbf{C}_{0h}}$.

3.4 On the solution of the subproblems from operator splitting

3.4.1 Solution of the advection subproblems

We solve the advection problem (3.3.63) by a wave-like equation method [4]. After translation and dilation on the time axis, each component of the velocity vector $\mathbf{u}$ and of the tensor $\mathbf{A}$ is solution of a transport equation of the following type:

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} + (\mathbf{U}\cdot\nabla)\varphi = 0 \text{ in } \Omega \times (t^n, t^{n+1}), \\ \varphi(0) = \varphi_0, \ \ \varphi = \mathbf{g} \text{ on } \Gamma^- \times (t^n, t^{n+1}), \end{cases} \tag{3.4.79}$$

where $\nabla \cdot \mathbf{U} = 0$ and $\dfrac{\partial \mathbf{U}}{\partial t} = 0$ on $\Omega \times (0, t)$. Thus, (3.4.79) is equivalent to the well-posed problem:

$$\begin{cases} \dfrac{\partial^2 \varphi}{\partial t^2} - \nabla \cdot ((\mathbf{U} \cdot \nabla \varphi)\mathbf{U}) = 0 \text{ in } \Omega \times (0, t), \\ \varphi(0) = \varphi_0, \ \ \dfrac{\partial \varphi}{\partial t}(0) = -\mathbf{U} \cdot \nabla \varphi_0, \ \ \varphi = \mathbf{g} \text{ on } \Gamma^- \times (t^n, t^{n+1}), \\ (\mathbf{U} \cdot \mathbf{n}) \left(\dfrac{\partial \varphi}{\partial t} + (\mathbf{U} \cdot \nabla)\varphi \right) = 0 \text{ on } \Gamma \setminus \Gamma^- \times (t^n, t^{n+1}). \end{cases} \tag{3.4.80}$$

Solving the wave-like equation (3.4.80) by a classical finite element/ time stepping method, a variational formulation of (3.4.80) is given by

$$\begin{cases} \displaystyle\int_\Omega \frac{\partial^2 \varphi}{\partial t^2} v \mathrm{d}\mathbf{x} + \int_\Omega (\mathbf{U} \cdot \nabla \varphi)(\mathbf{U} \cdot \nabla v) \mathrm{d}\mathbf{x} + \int_{\Gamma \setminus \Gamma^-} \mathbf{U} \cdot \mathbf{n} \frac{\partial \varphi}{\partial t} v \mathrm{d}\Gamma = 0, \forall v \in W_0, \\ \varphi(0) = \varphi_0, \ \ \dfrac{\partial \varphi}{\partial t}(0) = -\mathbf{U} \cdot \nabla \varphi_0, \ \ \varphi = \mathbf{g} \text{ on } \Gamma^- \times (t^n, t^{n+1}), \end{cases} \tag{3.4.81}$$

with the test function space W_0 defined by $W_0 = \{v | v \in H^1(\Omega), v = 0 \text{ on } \Gamma^-\}$.

Let H_h^1 be a C^0-conforming finite element subspace of $H^1(\Omega)$. We define $W_{0h} = H_h^1 \cap W_0$. We suppose that $\lim_{h \to 0} W_{0h} = W_0$ in the usual finite element sense. Next, we define $\boldsymbol{\tau}_1 > 0$ by $\boldsymbol{\tau}_1 = \dfrac{\triangle t}{Q}$ where Q is a positive integer, and we discretize problem (3.4.81) by

$$\begin{cases} \varphi^0 = \varphi_0, \\ \displaystyle\int_\Omega (\varphi^{-1} - \varphi^1) v \mathrm{d}\mathbf{x} = 2\boldsymbol{\tau}_1 \int_\Omega (\mathbf{U_h} \cdot \nabla \varphi^0) v \mathrm{d}\mathbf{x}, \ \forall v \in W_{0h}, \ \varphi^{-1} - \varphi^1 \in W_{0h}, \end{cases} \tag{3.4.82}$$

and for $q = 0, 1, 2, \cdots, Q-1$,

$$\begin{cases} \varphi^{q+1} \in H_h^1, \varphi^{q+1} = \mathbf{g}_h \text{ on } \Gamma^-, \\ \int_\Omega \frac{\varphi^{q+1} + \varphi^{q-1} - 2\varphi^q}{\tau^2} v \mathrm{d}\mathbf{x} + \int_\Omega (\mathbf{U_h} \cdot \nabla \varphi^q)(\mathbf{U_h} \cdot \nabla v) \mathrm{d}\mathbf{x} \\ \quad + \int_{\Gamma \setminus \Gamma^-} \mathbf{U_h} \cdot \mathbf{n} \left(\frac{\varphi^{q+1} - \varphi^{q-1}}{\tau} \right) v \mathrm{d}\Gamma = 0, \;\; \forall v \in W_0, \end{cases} \tag{3.4.83}$$

where $\mathbf{U}_h$ and $\mathbf{g}_h$ are the approximates of $\mathbf{U}$ and $\mathbf{g}$, respectively.

Remark 3.5. *Scheme* (3.4.82) – (3.4.83) *is a centreed scheme which is formally second order accurate with respect to space and time discretizations. To be stable, scheme* (3.4.82) – (3.4.83) *has to verify a condition such as* $\tau_1 \leq ch$*, which* c *of order of* $\frac{1}{\|\mathbf{U}\|}$*. Since the advection problem is decoupled from the other ones, we can choose proper time step here so that the above condition is satisfied. If one uses the trapezoidal rule to compute the first and the third integrals in* (3.4.83)*, the above scheme becomes explicit and* φ^{q+1} *is obtained via the solution of a linear system with diagonal matrix.*

Remark 3.6. *Scheme* (3.4.82) – (3.4.83) *does not introduce numerical dissipation, unlike the upwinding schemes commonly used to solve transport problems like* (3.4.79)*.*

Remark 3.7. *If we consider the homogeneous boundary condition,* $\mathbf{U}_h|_\Gamma = 0$ *and set* $Q = 1$ *in* (3.4.82) – (3.4.83)*. Then we obtain the following:*

$$\begin{cases} \int_\Omega \frac{\varphi^1 - \varphi^0}{\triangle t} v \, d\mathbf{x} + \int_\Omega (\mathbf{U_h} \cdot \nabla \varphi^0) v \, d\mathbf{x} \\ \quad = -\frac{\triangle t}{2} \int_\Omega (\mathbf{U_h} \cdot \nabla \varphi^0)(\mathbf{U_h} \cdot \nabla v) \, d\mathbf{x}, \;\; \forall v \in H_h^1; \varphi \in H_h^1 \end{cases} \tag{3.4.84}$$

3.4.2 Solution of the rigid body motion enforcement problems

In system (3.3.60)-(3.3.62), there are two multipliers. p and $\boldsymbol{\lambda}$. We have solved this system via an Uzawa-conjugate gradient method driven by both multipliers. The general problem is as follows:

Find $\mathbf{u} \in \mathbf{V}_{\mathbf{g}_{0h}}$, $p \in L^2_{0h}$, $\boldsymbol{\lambda} \in \Lambda_h$, $\mathbf{V} \in \mathbb{R}^3$, $\boldsymbol{\omega} \in \mathbb{R}^3$ such that

$$\begin{cases} -\int_\Omega p \nabla \cdot \mathbf{v}\, \mathrm{d}\mathbf{x} + \mu_f \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v}\, \mathrm{d}\mathbf{x} - \dfrac{\eta}{\lambda_1} \int_\Omega \mathbf{v} \cdot (\nabla \cdot (\mathbf{C} - \mathbf{I}))\, \mathrm{d}\mathbf{x} \\ +M_p \dfrac{\mathbf{V} - \mathbf{V}_0}{\triangle t} \cdot \mathbf{Y} + \mathbf{I_p} \dfrac{\boldsymbol{\omega} - \boldsymbol{\omega}_0}{\triangle t} \cdot \boldsymbol{\theta} \\ = \left(1 - \dfrac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} + \left\langle \boldsymbol{\lambda}, \mathbf{v} - \mathbf{Y} - \boldsymbol{\theta} \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \\ \quad \forall\, (\mathbf{v}, \mathbf{Y}, \boldsymbol{\theta}) \in \mathbf{V}_{0h} \times \mathbb{R}^3 \times \mathbb{R}^3, \end{cases} \tag{3.4.85}$$

$$\int_\Omega q \nabla \cdot \mathbf{u}\, \mathrm{d}\mathbf{x} = 0, \quad \forall q \in L^2_h, \tag{3.4.86}$$

$$\left\langle \boldsymbol{\mu}, \mathbf{u} - \mathbf{V} - \boldsymbol{\omega} \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h} = 0, \quad \forall \boldsymbol{\mu} \in \Lambda_h. \tag{3.4.87}$$

Applying the following Uzawa-conjugate gradient algorithm operating in the space $L^2_{0h} \times \Lambda_h$ to solve the sysyem (3.4.85)-(3.4.87):

Assume $p^0 \in L^2_{0h}$ and $\boldsymbol{\lambda}^0 \in \Lambda_h$ are given.

We solve the problem:

Find $\mathbf{u}^0 \in \mathbf{V}_{\mathbf{g}_{0h}}$, $\mathbf{V}^0 \in \mathbb{R}^3$, $\boldsymbol{\omega}^0 \in \mathbb{R}^3$ satisfying

$$\begin{cases} \mu_f \displaystyle\int_\Omega \nabla \mathbf{u}^0 : \nabla \mathbf{v}\, d\mathbf{x} = \int_\Omega p \nabla \cdot \mathbf{v}\, d\mathbf{x} + \frac{\eta}{\lambda_1} \int_\Omega \mathbf{v} \cdot (\nabla \cdot (\mathbf{C} - \mathbf{I}))\, d\mathbf{x} + \left\langle \boldsymbol{\lambda}^0, \mathbf{v} \right\rangle_{\Lambda_h}, \\ \forall\ \mathbf{v} \in \mathbf{V}_{0h}; \mathbf{u}^0 \in \mathbf{V}_{\mathbf{g}_{0h}}, \end{cases} \tag{3.4.88}$$

$$M_p \frac{\mathbf{V}^0 - \mathbf{V}_0}{\triangle t} \cdot \mathbf{Y} = \left(1 - \frac{\rho_f}{\rho_s}\right) M_p \mathbf{g} \cdot \mathbf{Y} - \left\langle \boldsymbol{\lambda}^0, \mathbf{Y} \right\rangle_{\Lambda_h}, \quad \forall\ \mathbf{Y} \in \mathbb{R}^3, \tag{3.4.89}$$

$$\mathbf{I_p} \frac{\boldsymbol{\omega}^0 - \boldsymbol{\omega}_0}{\triangle t} \cdot \boldsymbol{\theta} = -\left\langle \boldsymbol{\lambda}^0, \boldsymbol{\theta} \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\theta} \in \mathbb{R}^3, \tag{3.4.90}$$

and then compute

$$\mathrm{g}_1^0 = \nabla \cdot \mathbf{u}^0; \tag{3.4.91}$$

next find $\mathbf{g}_2^0 \in \Lambda_h$ *satisfying*

$$\left\langle \boldsymbol{\mu}, \mathbf{g}_2^0 \right\rangle_{\Lambda_h} = \left\langle \boldsymbol{\mu}, \mathbf{u}^0 - \mathbf{V}^0 - \boldsymbol{\omega}^0 \times \overrightarrow{\mathbf{Gx}} \right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\mu} \in \Lambda_h, \tag{3.4.92}$$

and set

$$\mathrm{w}_1^0 = \mathrm{g}_1^0, \quad \mathbf{w}_2^0 = \mathbf{g}_2^0. \tag{3.4.93}$$

Then for $k \geq 0$*, assuming that* p^k, $\boldsymbol{\lambda}^k$, $\mathbf{u}^k$, $\mathbf{V}^k$, $\boldsymbol{\omega}^k$, $\mathrm{g}_1^{\mathrm{k}}$, $\mathbf{g}_2^k$, w_1^k *and* $\mathbf{w}_2^k$ *are known, compute* p^{k+1}, $\boldsymbol{\lambda}^{k+1}$, $\mathbf{u}^{k+1}$, $\mathbf{V}^{k+1}$, $\boldsymbol{\omega}^{k+1}$, $\mathrm{g}_1^{\mathrm{k+1}}$, $\mathbf{g}_2^{k+1}$, ${\mathrm{w}_1}^{k+1}$ *and* $\mathbf{w}_2^{k+1}$ *as follows:*

$$\begin{cases} \mu_f \displaystyle\int_\Omega \nabla \overline{\mathbf{u}}^k : \nabla \mathbf{v}\, d\mathbf{x} = \int_\Omega \mathrm{w}_1^k \nabla \cdot \mathbf{v}\, d\mathbf{x} + \left\langle \mathbf{w}_2^k, \mathbf{v} \right\rangle_{\Lambda_h}, \\ \forall\ \mathbf{v} \in \mathbf{V}_{0h}; \overline{\mathbf{u}}^k \in \mathbf{V}_{\mathbf{g}_{0h}}, \end{cases} \tag{3.4.94}$$

$$M_p \frac{\overline{\mathbf{V}}^k}{\triangle t} \cdot \mathbf{Y} = -\left\langle \mathbf{w}_2^k, \mathbf{Y} \right\rangle_{\Lambda_h}, \quad \forall\ \mathbf{Y} \in \mathbb{R}^3, \tag{3.4.95}$$

$$\mathbf{I_p}\frac{\overline{\boldsymbol{\omega}}^k}{\triangle t}\cdot\boldsymbol{\theta} = -\left\langle \mathbf{w}_2^k, \boldsymbol{\theta}\times\overrightarrow{\mathbf{Gx}}\right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\theta}\in\mathbb{R}^3, \tag{3.4.96}$$

and then compute

$$\overline{\mathrm{g}}_1^{\mathrm{k}} = \nabla\cdot\overline{\mathbf{u}}^{\mathrm{k}}; \tag{3.4.97}$$

next find $\overline{\mathbf{g}}_2^k \in \Lambda_h$ *satisfying*

$$\left\langle \boldsymbol{\mu}, \overline{\mathbf{g}}_2^k\right\rangle_{\Lambda_h} = \left\langle \boldsymbol{\mu}, \overline{\mathbf{u}}^k - \overline{\mathbf{V}}^k - \overline{\boldsymbol{\omega}}^k\times\overrightarrow{\mathbf{Gx}}\right\rangle_{\Lambda_h}, \quad \forall\ \boldsymbol{\mu}\in\Lambda_h, \tag{3.4.98}$$

and compute

$$\rho_k = \frac{\displaystyle\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^k, \mathbf{g}_2^k\right\rangle_{\Lambda_h}}{\displaystyle\int_\Omega \overline{\mathbf{g}}_1^k \mathrm{w}_1^k\, d\mathbf{x} + \left\langle \overline{\mathbf{g}}_2^k, \mathbf{w}_2^k\right\rangle_{\Lambda_h}}, \tag{3.4.99}$$

and

$$p^{k+1} = p^k - \rho_k {\mathrm{w}_1}^k, \tag{3.4.100}$$

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k - \rho_k\mathbf{w}_2^k, \tag{3.4.101}$$

$$\mathbf{u}^{k+1} = \mathbf{u}^k - \rho_k\overline{\mathbf{u}}^k, \tag{3.4.102}$$

$$\mathbf{V}^{k+1} = \mathbf{V}^k - \rho_k\overline{\mathbf{V}}^k, \tag{3.4.103}$$

$$\boldsymbol{\omega}^{k+1} = \boldsymbol{\omega}^k - \rho_k\overline{\boldsymbol{\omega}}^k, \tag{3.4.104}$$

$$\mathrm{g}_1^{k+1} = \mathrm{g}_1^k - \rho_k\overline{\mathrm{g}}_1^k, \tag{3.4.105}$$

$$\mathbf{g}_2^{k+1} = \mathbf{g}_2^k - \rho_k\overline{\mathbf{g}}_2^k. \tag{3.4.106}$$

If

$$\frac{\displaystyle\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}+1}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{k+1}, \mathbf{g}_2^{k+1} \right\rangle_{\Lambda_h}}{\displaystyle\int_\Omega \left|\mathrm{g}_1^{0}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{0}, \mathbf{g}_2^{0} \right\rangle_{\Lambda_h}} \leq \varepsilon, \tag{3.4.107}$$

then take $p = p^{k+1}$*,* $\boldsymbol{\lambda} = \boldsymbol{\lambda}^{k+1}$*,* $\mathbf{u} = \mathbf{u}^{k+1}$*,* $\mathbf{V} = \mathbf{V}^{k+1}$*, and* $\boldsymbol{\omega} = \boldsymbol{\omega}^{k+1}$*. Otherwise, compute*

$$\gamma_k = \frac{\displaystyle\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}+1}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{k+1}, \mathbf{g}_2^{k+1} \right\rangle_{\Lambda_h}}{\displaystyle\int_\Omega \left|\mathrm{g}_1^{\mathrm{k}}\right|^2 d\mathbf{x} + \left\langle \mathbf{g}_2^{k}, \mathbf{g}_2^{k} \right\rangle_{\Lambda_h}}, \tag{3.4.108}$$

and set

$$\mathrm{w}_1^{k+1} = \mathrm{g}_1^{k+1} + \gamma_k {\mathrm{w}_1}^k, \tag{3.4.109}$$

$$\mathbf{w}_2^{k+1} = \mathbf{g}_2^{k+1} + \gamma_k \mathbf{w}_2^k. \tag{3.4.110}$$

Then do $m = m + 1$ *and go back to* (3.4.94).

3.5 Numerical results

3.5.1 Rotation of a single particle

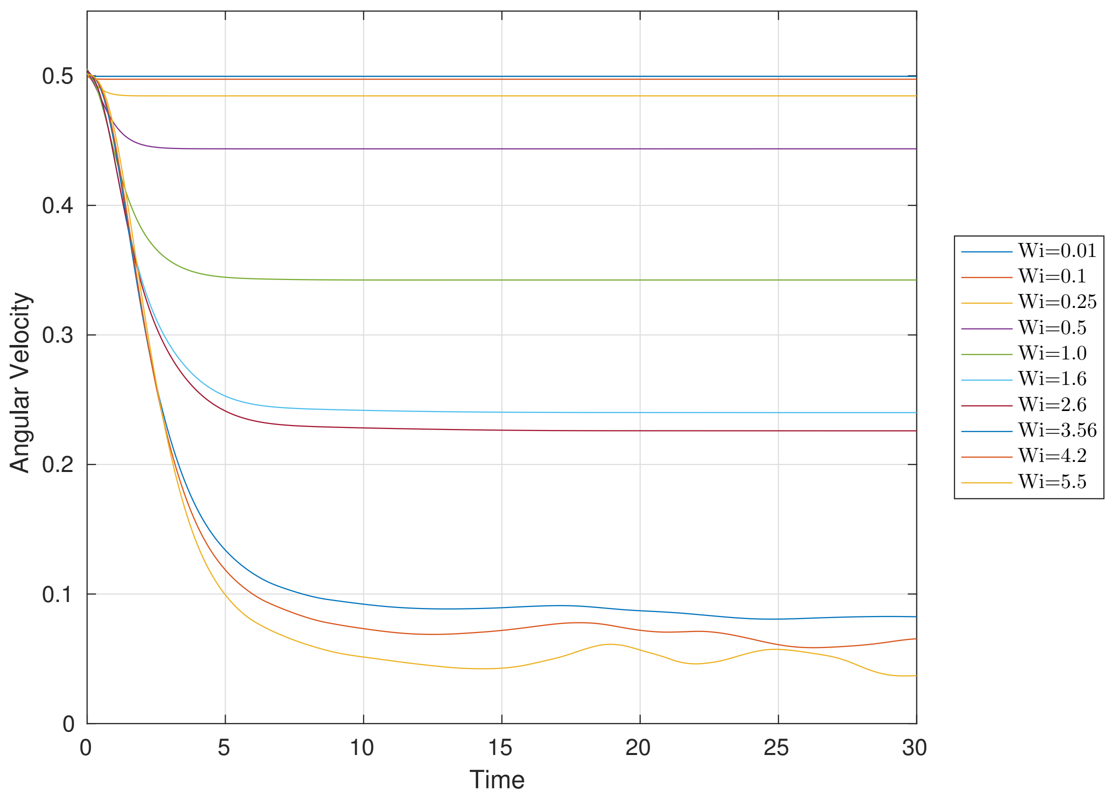
We have considered the cases of a single neutrally buoyant ball placed at the middle between two walls initially with respect to relaxation time λ_1 in a bounded shear flow of Oldroyd-B fluids. The densities of the fluid and that of the particle are $\rho_f = \rho_s = 1$ and the viscosity $\mu_f = 1$. The computational domain is $\Omega = (-x_1, x_1) \times (-x_2, x_2) \times (-x_3, x_3)$(i.e.,$L_1 = 2x_1, L_2 = 2x_2$, and $L_3 = 2x_3$).The shear rate $\dot{\gamma} = 1$ sec^{-1} so the velocity of the top wall is $U = x_3$ and the velocity of the bottom wall is $-U = -x_3$.

For all the numerical simulations, we assume that all dimensional quantities are in the CGS units. We have obtained the rotating angular velocity with respect to the x_2-axis for different values of λ_1 with the retardation time $\lambda_2 = \lambda_1/8$.

First, to study the slowing down effect in the particle rotating angular velocity due to a finite wall-particle distance, we consider the mass center of the ball is fixed at $(0, 0, 0)$ with three different λ_1 and define the blockage ratio $K = 2r/L_3$ with five particle radii $r = 1/10, 1/5, 1/3, 2/5, 1/2$. The associated values of the Weissenberg number Wi ($= \lambda_1\dot{\gamma}$) are $0.5, 0.75$, and 1.0. In order to assure the unpertubed conditions, the computational domain is $\Omega = (-L/2, L/2) \times (-L/2, L/2) \times (-1, 1)$ where $L = 20r$ and $L_3 = 2$. So we can consider five different block ratios K as same as those cases in [5] for the numerical results.

graph????

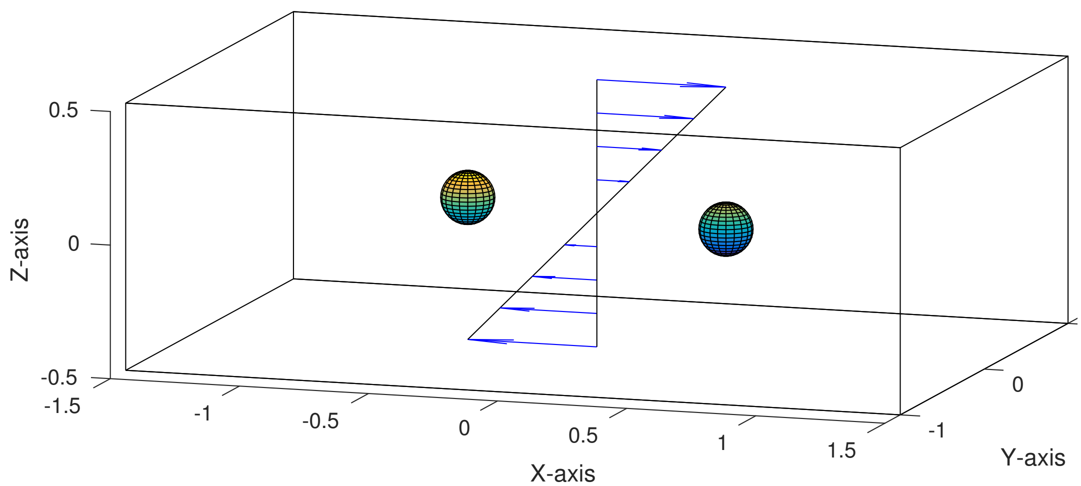
Second, to study the effect of viscoelasticity in the particle rotating angular velocity, we consider two different setups of mass center. First one is the cases of particle with fixed mass center at $(0, 0, 0)$ all the time and the second one is the case of free moving particle without fixed mass center. The particle radius r is 0.1. The computational domain is $\Omega = (-1.5, 1.5) \times (-1.5, 1.5) \times (-1.5, 1.5)$. The mass center of the ball is located at $(0, 0, 0)$ initially. We have obtained the rotating angular velocity with respect to the x_2-axis for ten different values of the relaxation time λ_1 with the retardation time $\lambda_2 = \lambda_1/8$. The associated values of the Weissenberg number Wi ($= \lambda_1\dot{\gamma}$) are 0.01, 0.1, 0.25, 0.5, 1, 1.6, 2.6, 3.56, 4.2, and 5.5.



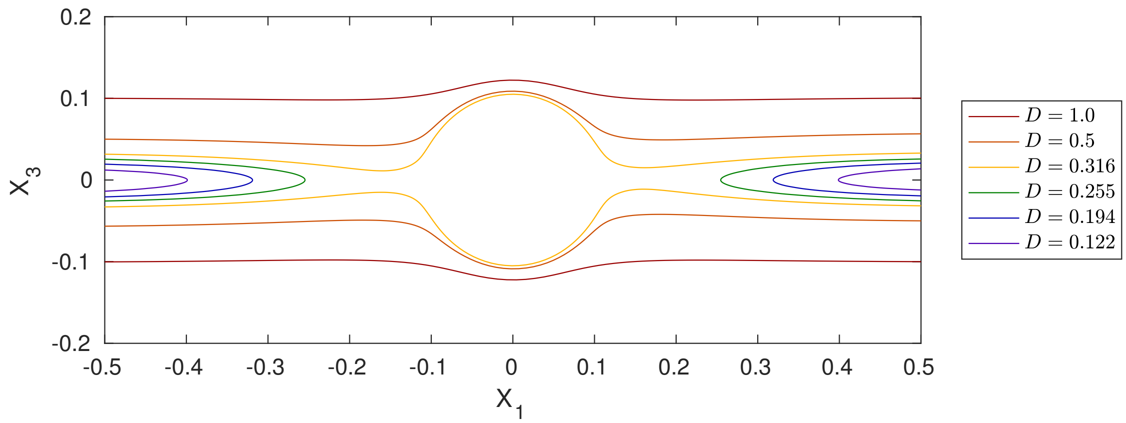
Angular Velocity
Time
0
0.1
0.2
0.3
0.4
0.5
0
5
10
15
20
25
30
Wi=0.01
Wi=0.1
Wi=0.25
Wi=0.5
Wi=1.0
Wi=1.6
Wi=2.6
Wi=3.56
Wi=4.2
Wi=5.5

3.5.2 Migration of a single particle in an one wall driven bounded shear flow

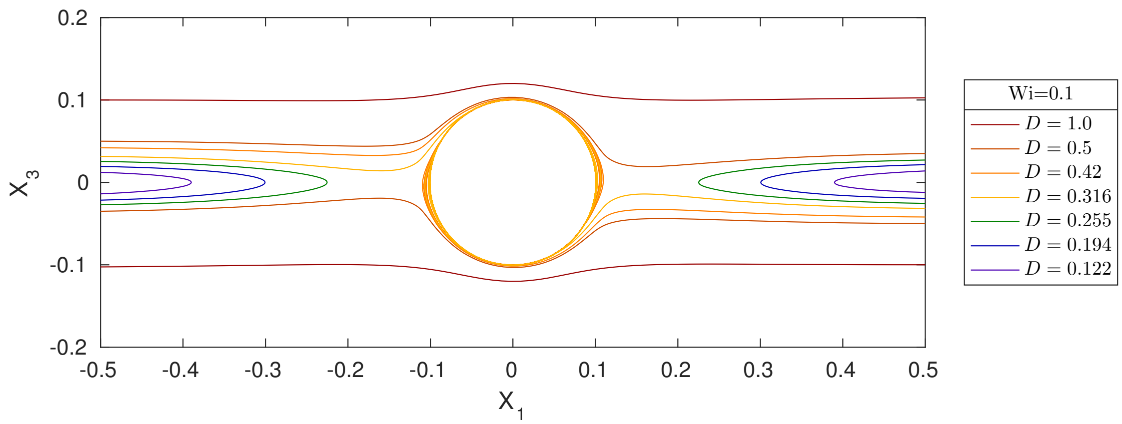
3.5.3 Two ball interacting with large initial distance in a two wall driven bounded shear flow

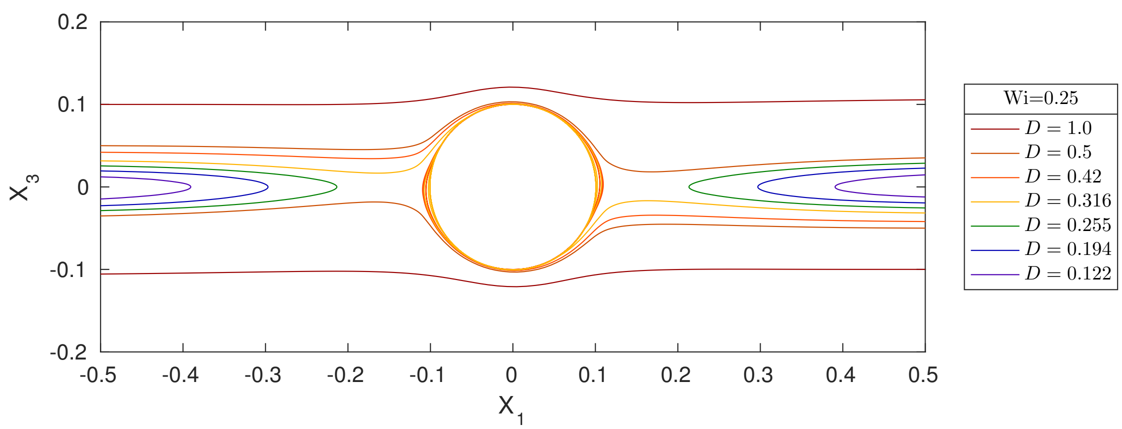


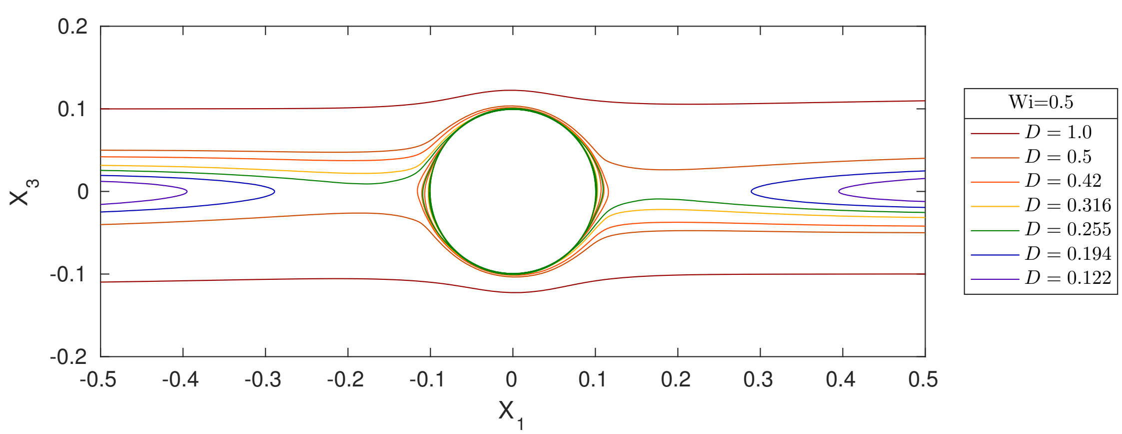
In this section we consider the cases of two balls of the same size interacting in a bounded shear flow fluid of Oldroyd-B type as visualized in Fig. ??. The ball radii are $r = 0.1$. The fluid and ball densities are $\rho_f = \rho_s = 1$, the viscosity being $\mu = 1$. The computational domain is $\Omega = (-1.5, 1.5) \times (-1, 1) \times (-0.5, 0.5)$ (i.e., $L_1 = 3$, $L_2 = 2$, and $L_3 = 1$). The shear rate is fixed at $\dot{\gamma} = 1$ so the velocity of the top wall is $U = 0.5$, the bottom wall being $U = -0.5$. The mass centers of the two balls are located on the shear plane at $(-d_0, 0, \triangle s)$ and $(d_0, 0, -\triangle s)$ initially, where $\triangle s$ varies and d_0 is 0.5. The time step being $\triangle t = 0.001$. Then we consider six or seven dimensionless initial vertical displacements $D = \triangle s/a$ from the ball center to the middle plane in the two wall driven bounded shear flow.

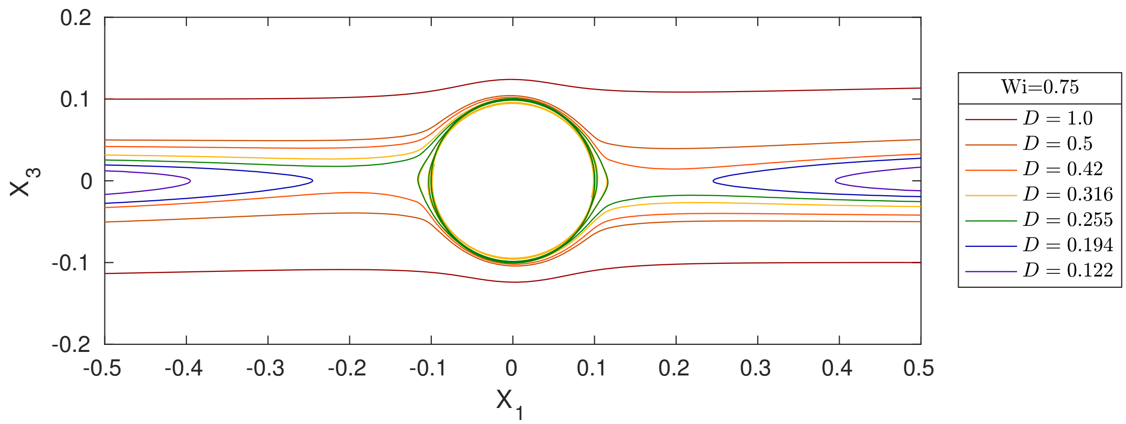


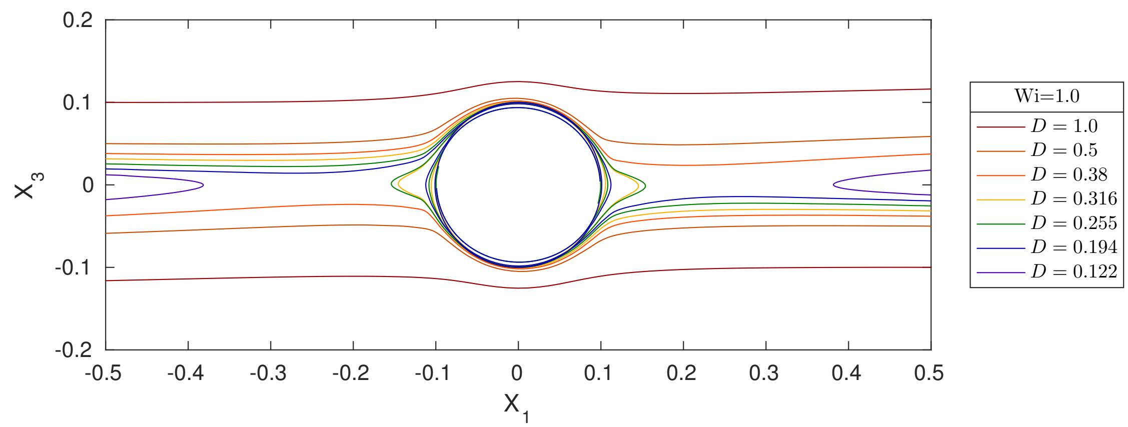
When two balls move in a bounded shear flow of a Newtonian fluid at Stokes regime with D = 0.122, 0.194, 0.255, 0.316, 0.5, 1 as in Fig. **??**, the higher ball takes over the lower one and then both return to their initial heights for those large vertical displacements D = 0.316, 0.5 and 1. These two 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 two particle paths are called return trajectories. Both kinds are on the shear plane as shown in Fig. **??** for Wi=0 (Newtonian case) and they are consistent with the results obtained in [21].


0.2
0.1
0
-0.1
-0.2
X_3
-0.5 -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5
X_1
Wi=0.1
$D = 1.0$
$D = 0.5$
$D = 0.42$
$D = 0.316$
$D = 0.255$
$D = 0.194$
$D = 0.122$

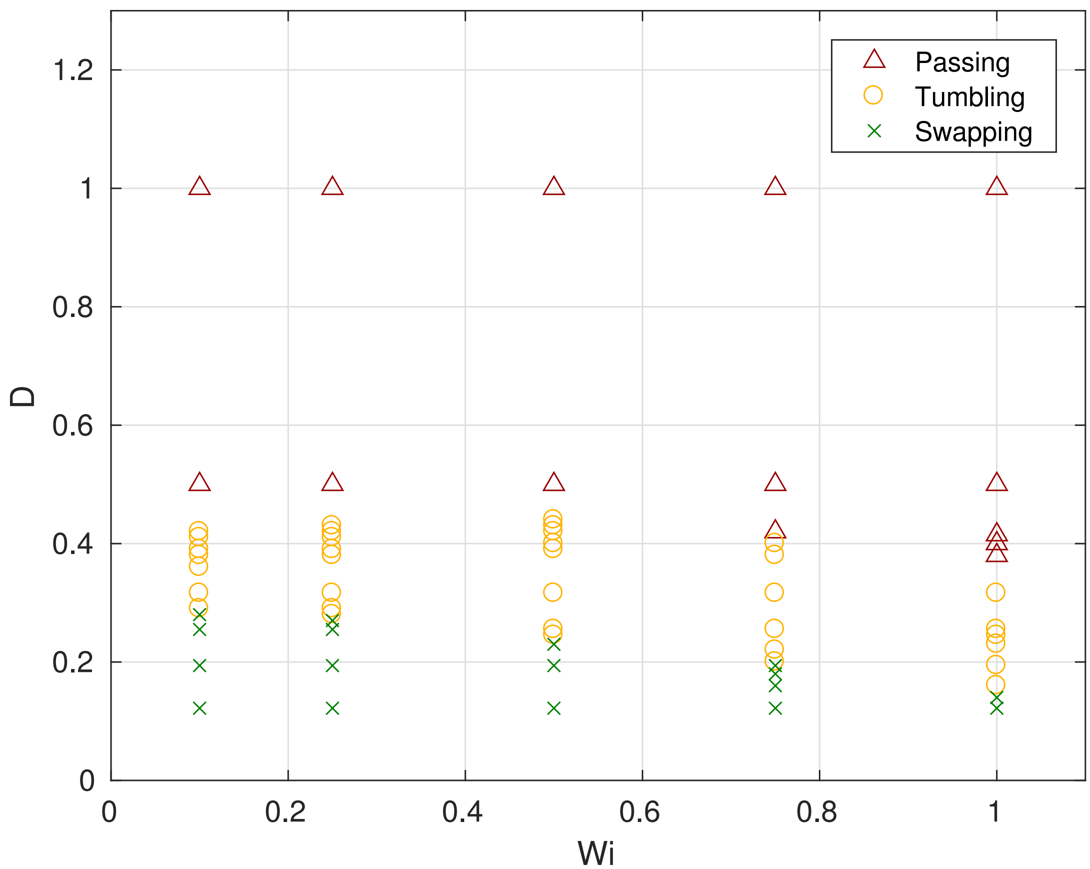

0.2
0.1
0
-0.1
-0.2
X_3
-0.5 -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5
X_1
Wi=0.25
$D = 1.0$
$D = 0.5$
$D = 0.42$
$D = 0.316$
$D = 0.255$
$D = 0.194$
$D = 0.122$


0.2
0.1
0
-0.1
-0.2
X_3
-0.5 -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5
X_1
Wi=0.5
$D = 1.0$
$D = 0.5$
$D = 0.42$
$D = 0.316$
$D = 0.255$
$D = 0.194$
$D = 0.122$

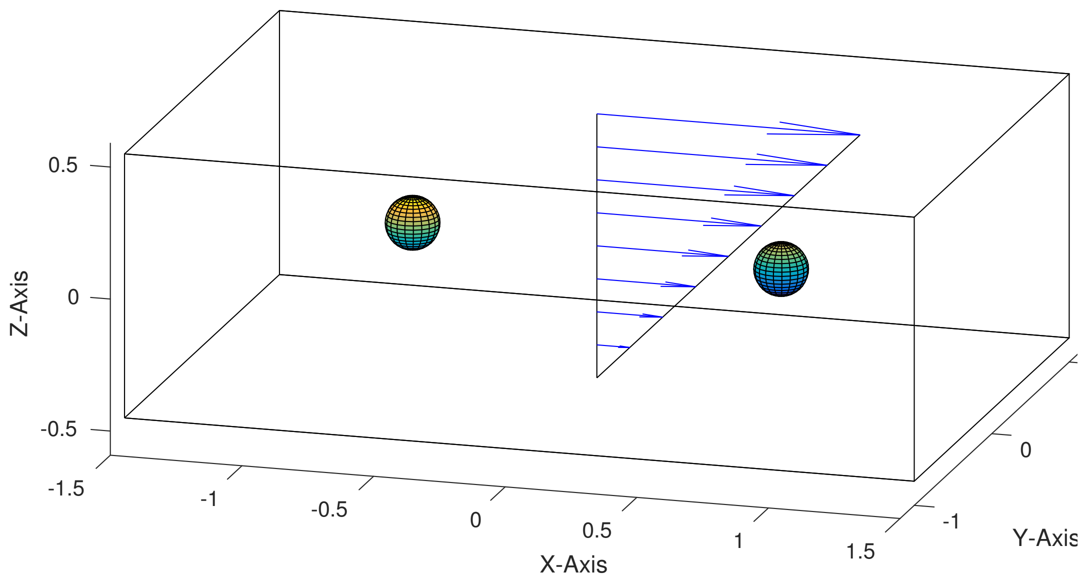




For the two balls interacting in an Oldroyd-B fluid with $D = 0.122$, 0.194, 0.255, 0.316, 0.42, 0.5, 1 , we have summarized the results for Wi=0.1, 0.25, 0.5, 0.75, and 1 in Figs. **??** to **??**. As in Newtonian fluids, there are results of pass and return trajectories concerning two ball encounters; but the those 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 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 change the shape of the trajectories. For higher values of Wi considered in this section, there are less return trajectories; instead it is easier to obtain the two ball chain once they run into each other. Actually depending on the Weissenberg number Wi and the initial vertical displacement $\triangle s$, a chain of two balls can be formed in a bounded shear flow, and then such chain tumbles. For example, for $D = 0.316$, the two balls come to each other, form a chain and then rotate with respect to the midpoint between two mass centers for Wi=0.1, 0.25, 0.5, and 1. The details of the phase diagram of pass, return, and tumbling are shown in Fig. **??**. The range of the vertical distance for the passing over becomes bigger for higher Weissenberg numbers. For the shear flow considered in this article, the increasing of the value of the Wi with a fixed shear rate is same as to increase the shear rate with a fixed relaxation time. This explains why, for Wi=1, two balls can have bigger gap between them while rotating with respect to the middle point between two mass centers since the two balls are kind of moving under higher shear rate. Those tumbling trajectories are associated with the closed streamlines around a freely rotating ball centred at the origin.

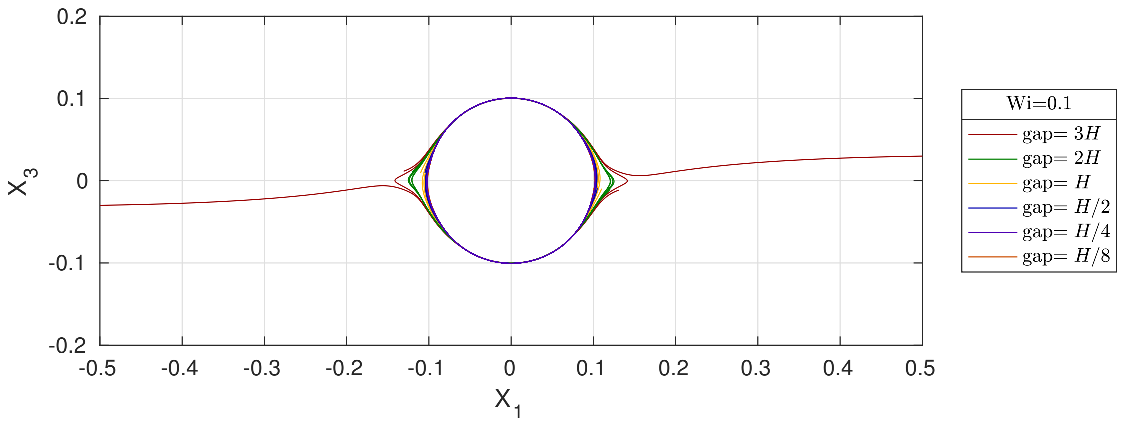

Passing
Tumbling
Swapping
D
Wi
0
0.2
0.4
0.6
0.8
1
1.2

3.5.4 Two ball interacting with small initial distance in an one wall driven bounded shear flow

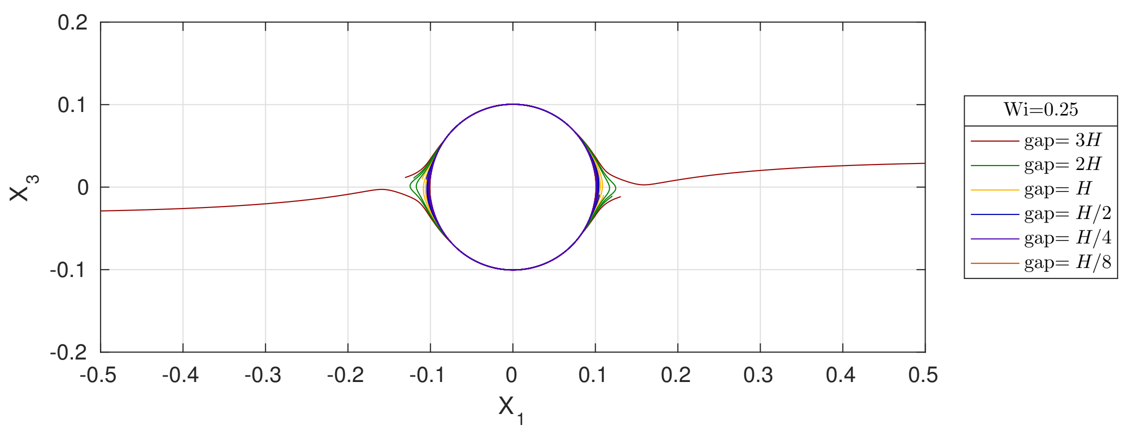


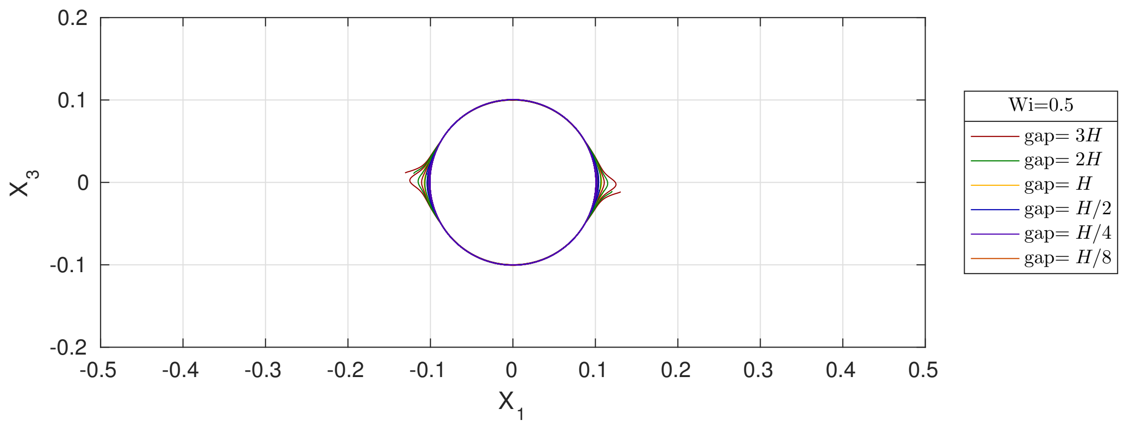
In this section we consider the cases of two balls of the same size interacting in a bounded shear flow driven by the upper wall as visualized in Fig. ??. The ball radii are $r = 0.1$. The fluid and ball densities are $\rho_f = \rho_s = 1$, the viscosity being $\mu = 1$. The computational domain is $\Omega = (-1.5, 1.5) \times (-1, 1) \times (-0.5, 0.5)$. The shear rate is fixed at $\dot{\gamma} = 1$ but the velocity of the top wall is $U = 1$, the bottom wall being $U = 0$. 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 $\triangle t = 0.001$. The mass centers of the two balls are located on the shear plane at $(-x_0, 0, z_0)$ and $(x_0, 0, -z_0)$ initially such that the angle between the mid-plane and the line segment of two initial locations of mass center of particle is 175° counterclockwisely. We define the gap size

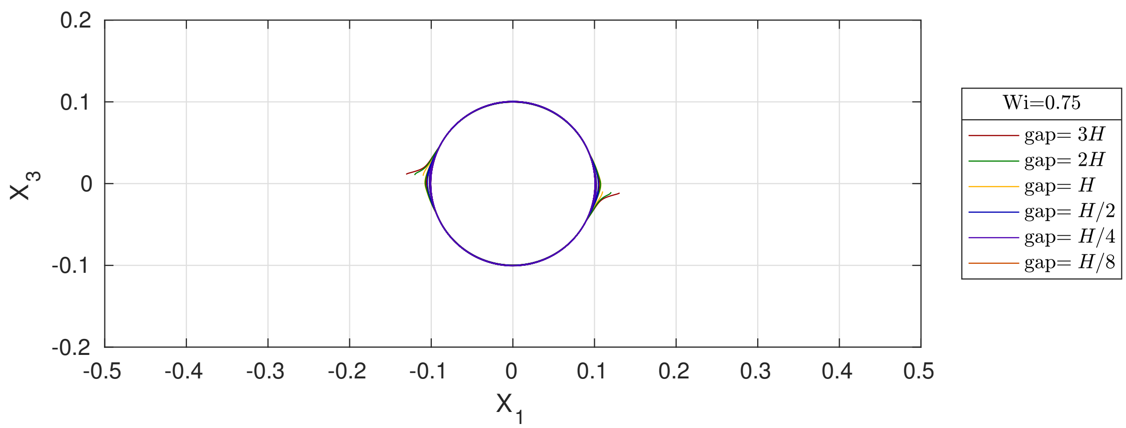
$= d - 2r$ where d is the distance between two mass centers of particle and r is 0.1.

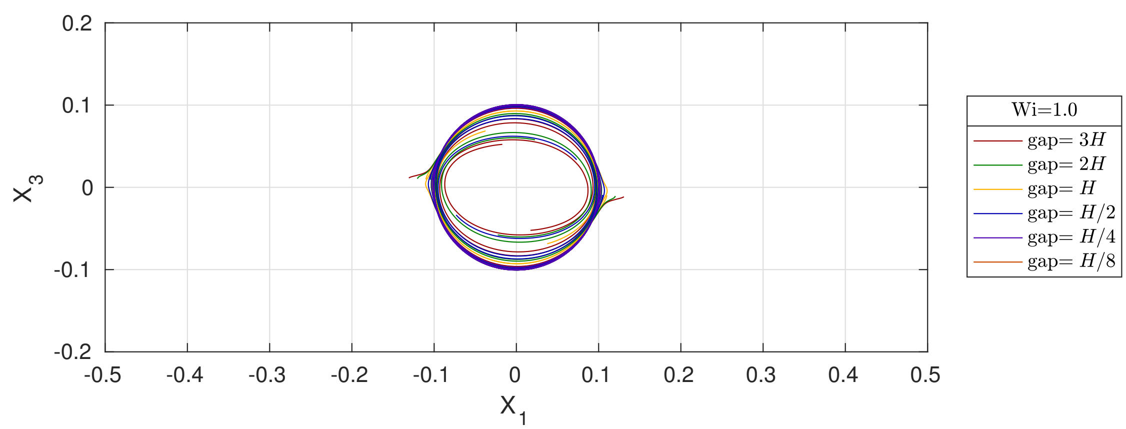


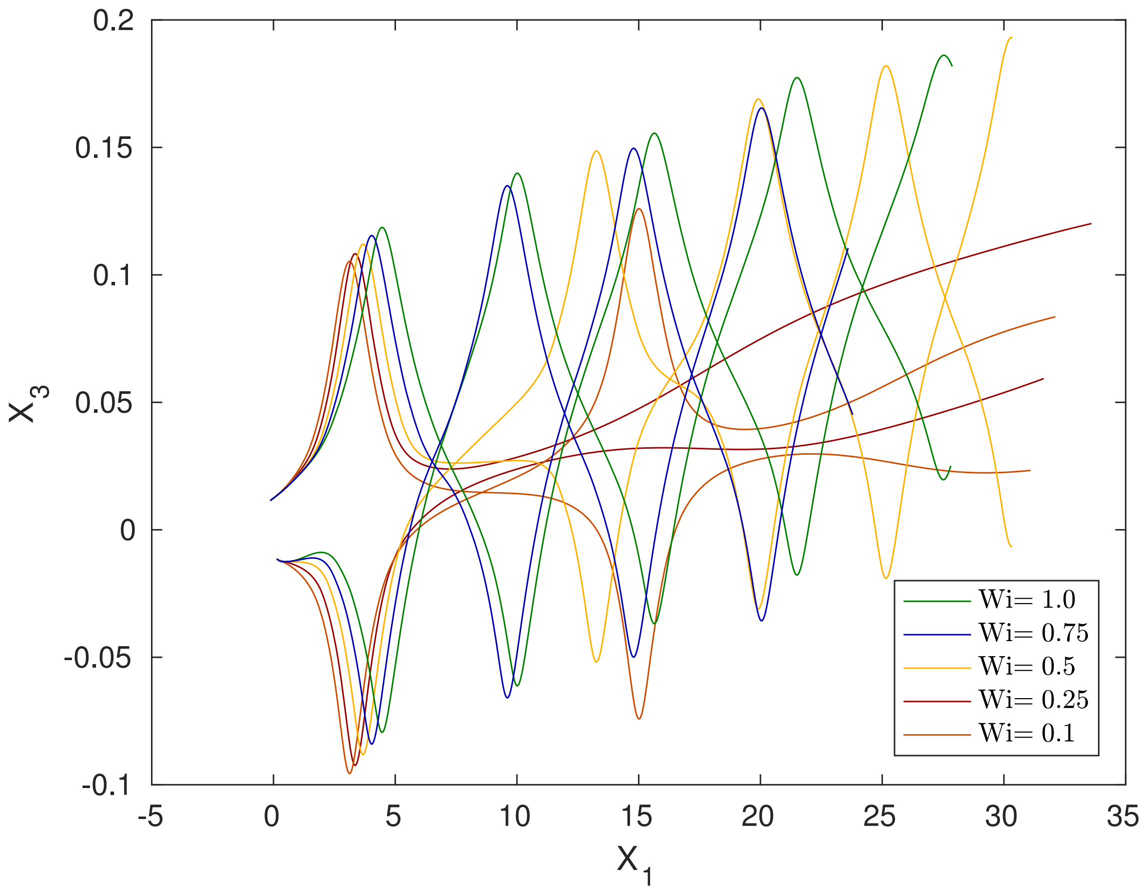
For the two balls interacting in Oldroyd-B fluid with gap= $h/8$, $h/4$, $h/2$, h, $2h$, and $3h$ where h is the mesh size, we have summarized the results for Wi=0.1, 0.25, 0.5, 0.75, and 1 in Figs. **??** to **??**.

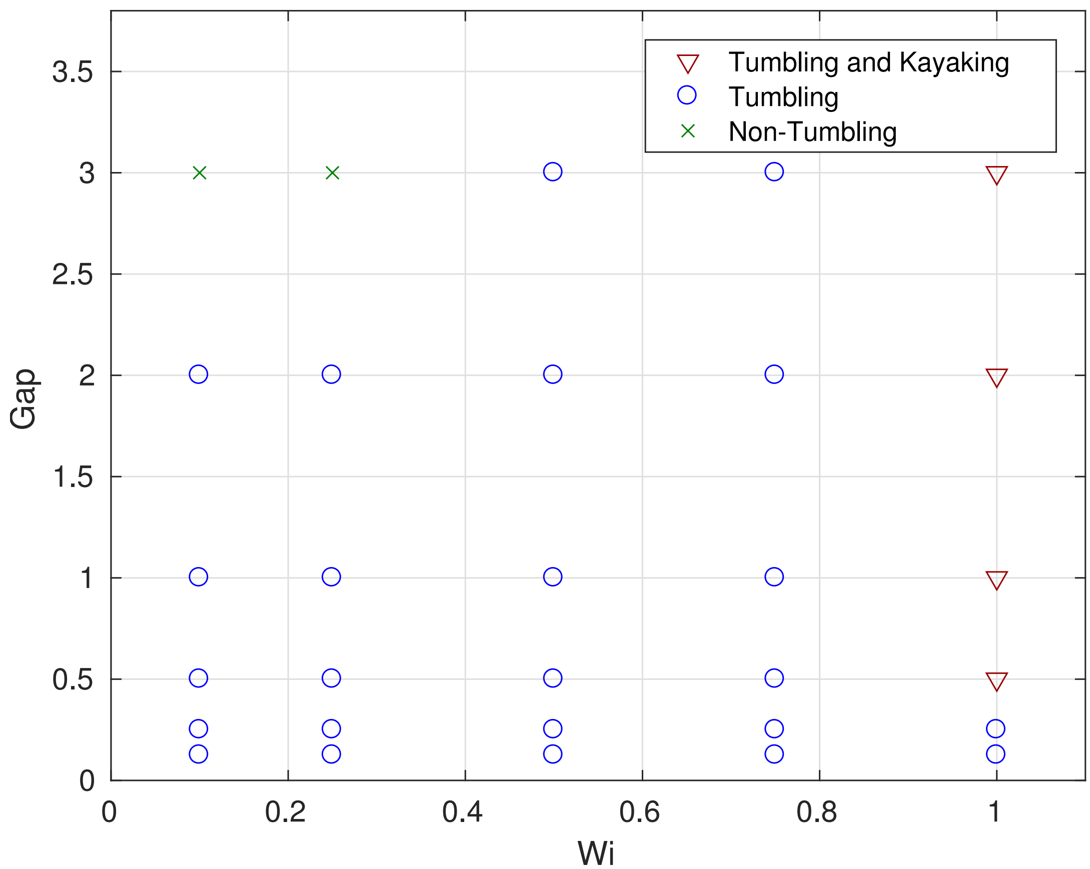



0.2
0.1
0
-0.1
-0.2
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
X_3
X_1
Wi=0.5
gap= $3H$
gap= $2H$
gap= H
gap= $H/2$
gap= $H/4$
gap= $H/8$


0.2
0.1
0
-0.1
-0.2
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
X_3
X_1
Wi=0.75
gap= $3H$
gap= $2H$
gap= H
gap= $H/2$
gap= $H/4$
gap= $H/8$


0.2
0.1
0
-0.1
-0.2
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
X_3
X_1
Wi=1.0
gap= $3H$
gap= $2H$
gap= H
gap= $H/2$
gap= $H/4$
gap= $H/8$


0.2
0.15
0.1
0.05
0
-0.05
-0.1
-5
0
5
10
15
20
25
30
35
X3
X1
Wi= 1.0
Wi= 0.75
Wi= 0.5
Wi= 0.25
Wi= 0.1


Tumbling and Kayaking
Tumbling
Non-Tumbling
Gap
Wi
0
0.5
1
1.5
2
2.5
3
3.5
0
0.2
0.4
0.6
0.8
1

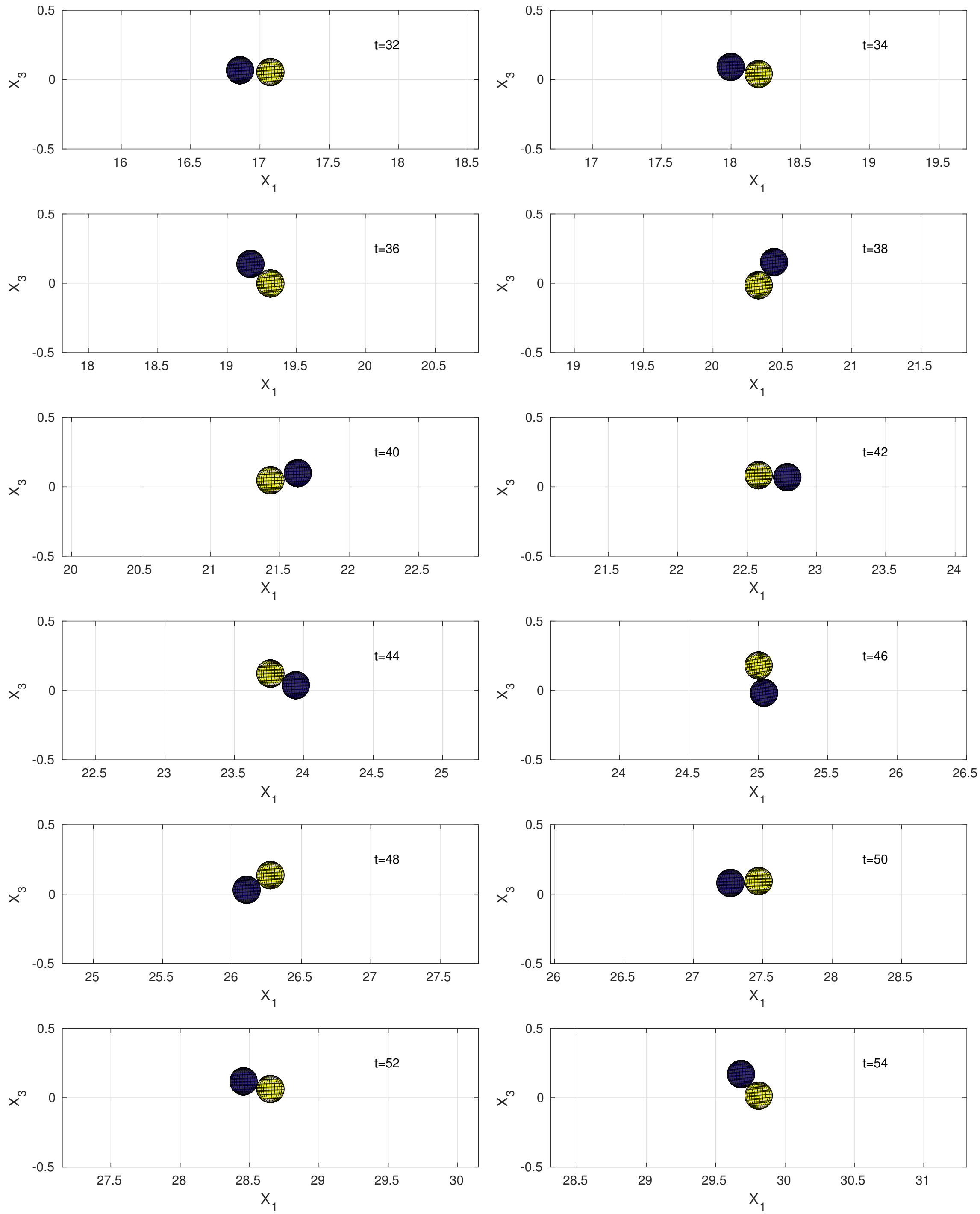


Figure 3.5.1: The tumbling motion as $Wi = 0.5$: the initial distance between two particles is 2r+gap where $r = 0.1$, gap=$3h$.For each frame, the horizontal direction is X_1 axis and vertical direction is X_3 axis.

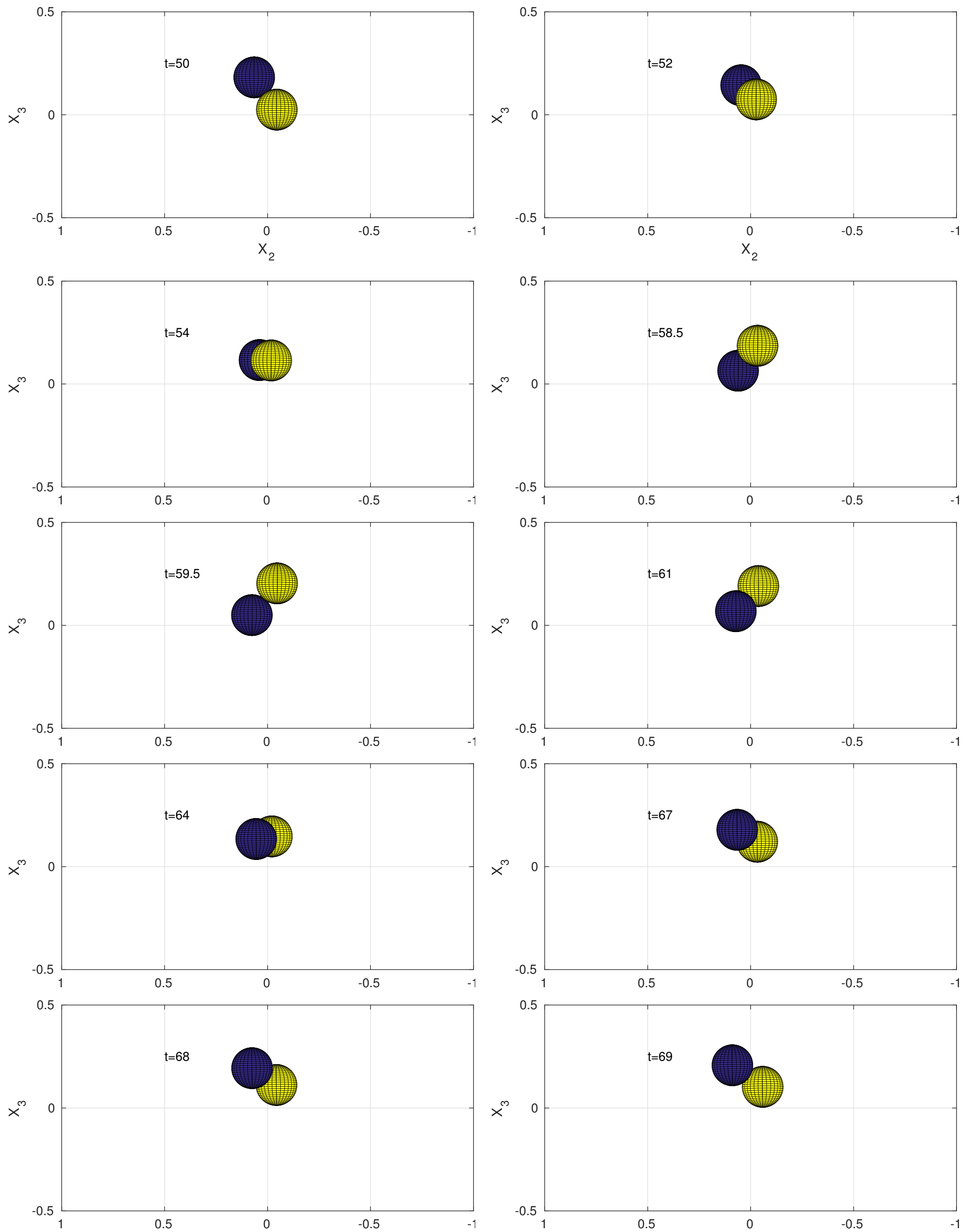


Figure 3.5.2: The kayaking motion as $Wi = 1.0$: the initial distance between two particles is 2r+gap where $r = 0.1$, gap=$3h$. For each frame, the horizontal direction is X_2 axis and vertical direction is X_3 axis.

CHAPTER 4

Concluions and Future work

4.1 Concluions

4.2 Future work

The particles chain phenomenon in non-Newtonian shear flow has been observed experimentally in [12] and [18]. The numerical model of three particles alignment in a viscoelastic fluid has been introduced in [9]. However, the numerical simulation of particle-chains in non-Newtonian shear flow haven't been developed. I will use the

Oldroyd-B fluid with shear thinning to investigate the chain phenomenon of many particles with random initial positions.

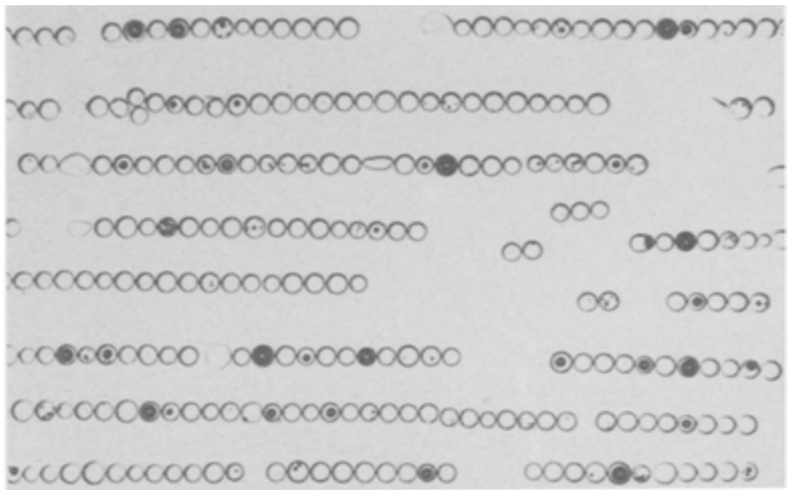


Figure 4.2.1: Particles alignment in polyisobutylene solution(J. Michele et al. Rheol. Acta 1977)

Another extension of my current work will be the finitely extensible nonlinear elastic (FENE) dumbbell model in non-Newtonian fluid flow. In order to study the properties of dilute polymer fluid, the motion of polymer molecules in the fluid is modeled as a suspension of dumbbells or spring chains with finite extensibility (e.g., see [1] and [2]). Besides the typical topics, such as the flow in the channel, flow in a cross-slot geometry and impacting drop problem, it would be interesting to consider the fluid-particle and particle-particle interactions in non-Newtonian fluid flow of FENE type with particles.

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