Computing of Dynamics of Soft Particles using Front-Tracking Method

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Abstract. The dynamics of droplets and elastic capsules in a low Reynolds number flow is investigated by Front-Tracking method. The motions of droplets under gravity field, shear flow and Poiseuille flow are shown as examples. The capsules are migrated to the center line of the Poiseuille flow due to the lateral migration. The hydrodynamic conductance of the Poiseuille flow is reduced as the capsule goes to the center of the channel. The small capsules move to the boundary wall of the Poiseuille flow in the mixture of large and small capsules.

1. Introduction
The motion of deformable particles, such as droplets, vesicles and capsules, is becoming one of the most remarkable study. The simulation of the deformable particles are well presented in various literatures[1, 2, 3]. The study of the motion of deformable particles provides us useful information for the development of a Drug Delivery System (DDS). The suction of a droplet from simple shear flow region to Poiseuille flow region has been dealt with in our previous paper [4], as shown in Fig. 1. We have elucidated the criterion of the suction for the enhancement of the efficiency of drug transportation to the diseased part.

In general, the DDS particle flows in the blood vessel dispersed with red blood cells, white blood cells, platelets, and so on. The DDS particle we consider is smaller than the red blood cell. The blood cell has a tendency to move to the center of the vessel because of the lateral migration. As a consequence, the DDS particle is anticipated to be pushed out from the central region toward the periphery of the blood vessel. Then the DDS particle will be more easily sucked into the cleft of the vessel to cure the inflamed part.

In this paper, a simulation of the deformable particles under gravity or pressure gradient field is shown. In the simulation, the finite difference method and Front-Tracking method are used. The method was developed by Peskin et al.[5, 6, 7, 8] and was applied for droplet migration problems by Tryggvason et al.[9, 10, 11, 12, 13, 14, 15, 16, 17]. The Front-Tracking method uses two types of mesh, Eulerian mesh and Lagrangian mesh. The Eulerian mesh is used to calculate the field data of velocity and pressure. The Lagrangian mesh describes the shape of deformable particles. Examples of the droplets under gravity, the droplets under shear field, and the elastic capsules in the Poiseuille flow are presented in this study.
Figure 1. Suction of a droplet from the shear region to the Poiseuille region.

Figure 2. Lagrangian mesh, which composes a particle shape, is immersed in Eulerian mesh.

2. Formulation
In this section, we describe the method of the computation of deformable particles in the Newtonian fluid.

A set of rectangular structured mesh (Eulerian mesh) for fluid computation and unstructured triangular mesh (Lagrangian mesh) for a deformable particle is prepared as shown in Fig. 2. In general, a density field and a viscosity field depend on whether the Eulerian mesh points are inside of the particle or outside of the particle.

The velocity field $v(r)$ and pressure field $p(r)$ of an incompressible fluid with density $\rho(r)$ and viscosity $\mu(r)$ are governed by the Navier-Stokes equation

$$\rho \left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) = -\nabla p + \nabla \cdot \mu(r) \left( \nabla v + (\nabla v)^t \right) + \rho g + f, \quad (1)$$

and the continuity equation

$$\nabla \cdot v = 0, \quad (2)$$
where $A^t$ denotes the transpose of tensor $A$, $g$ is a gravity acceleration and $f$ is the force acting from the interface of deformed particle. The fluid outside of the droplet has a viscosity $\mu(r) = \mu$ and a density $\rho(r) = \rho$, whereas the fluid inside the droplet has a viscosity $\mu(r) = \mu'$ and a density $\rho(r) = \rho + \Delta \rho$. The viscosity ratio $\lambda$ is defined as $\lambda = \mu'/\mu$.

The velocity and pressure are assigned on the Eulerian mesh point. The Highly Simplified Maker And Cell (HSMAC) method is used to solve the fluid fields. The time evolution of the front of the particles is calculated from the velocity on the surface. Because the mesh point (Lagrangian mesh) on the surface does not coincide with the field point (Eulerian mesh), the velocity $v_L$ on the surface is calculated from the field velocity $v_E$ as

$$v_L(r) = \sum w(r - r') v_E(r')$$  \hspace{1cm} (3)

where $w(r)$ is defined as

$$w(r - r') = d \left( \frac{r_x - r'_x}{\Delta x} \right) d \left( \frac{r_y - r'_y}{\Delta y} \right) d \left( \frac{r_z - r'_z}{\Delta z} \right),$$  \hspace{1cm} (4)

$\Delta x, \Delta y$ and $\Delta z$ are the sizes of the lattice for each direction, and Brackbill and Ruppel’s weight function [18]

$$d(r) = \begin{cases} \frac{2}{9}r^2 + \frac{1}{2}r^3, & 0 < r < 1 \\ \frac{2}{9}(2 - r)^3, & 1 \leq r \leq 2 \\ 0, & \text{otherwise} \end{cases}$$  \hspace{1cm} (5)

is used in our simulation.

On the other hand, the force density $f$ in eq. (1) is calculated by

$$f(r') = \sum w(r' - r) t(r) \frac{\Delta S}{\Delta x \Delta y \Delta z}$$  \hspace{1cm} (6)

where $t$ is a traction on the surface of the particle and $\Delta S$ is the area of the surface element.

The traction $t$ depends on the expression of the surface free energy. For a droplet with the surface tension coefficient $\sigma$, the surface free energy $F^d$ is

$$F^d = \sigma \int dS,$$  \hspace{1cm} (7)

where the integration is over the droplet surface. The traction is derived from the functional derivation

$$t = \frac{\delta F^d}{\delta r} = 2\sigma H n,$$  \hspace{1cm} (8)

where $H$ is the mean curvature and $n$ is a unit normal on the droplet.

For the elastic membrane with Young’s modulus $E$, the free energy $F^e$ is

$$F^e = \frac{E}{6} \int \left( \lambda_1^2 + \lambda_2^2 + \lambda_1^{-2}\lambda_2^{-2} - 3 \right) dS,$$  \hspace{1cm} (9)

where $\lambda_1$ and $\lambda_2$ are the square roots of eigen values of Cauchy-Green tensor. For the details, consult literatures [3] and [19].

The position $r(t + \Delta t)$ of the node on the particle surface is evolved by the Euler method

$$r(t + \Delta t) = r(t) + v(t) \Delta t.$$  \hspace{1cm} (10)

For the droplet, the mesh stabilization algorithm, which is described in a paper [20], is used. Figure 3 shows the efficiency of this algorithm. The connection of the nodes does not change, and the calculation is stable as shown in Fig. 3 (b).
Figure 3. Mesh stabilization for a droplet. Fig. 3(a) shows a simulation without the mesh stabilization. The nodes on the mesh flows toward the rear side of the droplet. Fig. 3(b) shows a simulation with the mesh stabilization.

Figure 4. Sedimentation of droplets. Bond number $Bo$ is 0.5 in (a) and 5 in (b).

3. Results
3.1. Sedimentation of droplets
The snapshots of the droplets under gravity with $Re = 23$ are shown in Fig. 4. The periodic boundary is used in this simulation. Bond number is defined as the ratio of the gravity to the surface tension $Bo = \Delta \rho g a^2 / \sigma$, where $\Delta \rho$ is the density difference between the bulk fluid and the droplet and $a$ is the radius of the droplet. When the Bond number is higher, the gravity effect is higher than the surface tension so that the droplet is more deformable. The droplets in Fig. 4(a) keep spherical shapes, whereas the droplets in Fig. 4(b) are deformed under gravity. The average position of the droplets against time is shown in Fig. 5. The time evolution of the average position for $Bo = 0.5$ and 5 are almost the same. The movement of the droplets is not remarkably dependent on the deformation in this case. The inserted triangle in Fig. 5 shows the analytical reduced velocity in the case of a zero Reynolds number flow without interaction and deformation

$$\frac{V}{a^2 \Delta \rho g \mu} = \frac{2(1 + \lambda)}{3(2 + 3\lambda)}$$  \hspace{1cm} (11)

which is known as Hadamard-Rybczinski result. Our results show the multi-droplets motion is slightly faster than the single ideal motion of a droplet.
Figure 5. Average of the centers $<|z|>/a$ of the droplet as a function of time $t\Delta \rho ag/\mu$. A slope of inserted triangle in the figure shows the reduced velocity for a single spherical droplet at $Re = 0$.

Figure 6. Shear induced motion of droplets. The distance between the centers of the droplets in the $y$ direction is $1.8a$ in (a) and $0.8a$ in (b).

3.2. Shear induced deformation of droplets
Two droplets under shear flow with shear rate $\dot{\gamma}$ are shown in Fig. 6. In this case, Capillary number is $Ca = \mu \dot{\gamma}a/\sigma = 0.1$ and the viscosity ratio $\lambda$ is 10. The initial distance between the centers of the droplets in the $y$ direction is $1.8a$ in (a) and $0.8a$ in (b). The deformation of the droplets in (b) is larger than those in (a).

3.3. Lateral migration
An elastic capsule, whose property is given in eq.(9) with $a^2E/p_x = 1.28 \times 10^4$, is placed in the Poiseuille flow between the two plates with the separation distance $l_y = 3.2a$, where $a$ is the radius of the capsule. The pressure gradient is $p_x$ in the $x$ direction and the Reynolds number $Re$ is 0.1. The periodic boundary condition is imposed on the $x$ and $z$ directions. We assume
the analytic solution of stable Poiseuille flow as an initial velocity profile. Figure 7 shows the snapshots of the elastic capsule whose initial position from the bottom plate is $1.1a$. The capsule moves to the center of the channel. This phenomenon is known as the lateral migration.

Figure 8 shows the time variation of the center of the capsule with different initial positions. Every capsule moves to the center of the channel.

The hydrodynamic conductance is shown in Fig. 9. The fluid flux $q$ is calculated by the integral of the $x$ component’s velocity $v_x$ over the cross section $S$ including inside the capsule, defined as

$$ q = \frac{1}{S} \int_S v_x dS. \quad (12) $$

The hydrodynamic conductance is defined as $\nu = q/p_x$. The conductance $\nu_0$ without capsules is $\nu_0 = l_0^2/(12\mu)$. Each line in Fig. 9 is calculated for different initial position of the capsule. The conductance is low in the case where the capsule is near the wall, but it is high when the capsule is located in the central region. Due to the lateral migration, the terminal conductance is independent of the initial position of the capsule.

Finally, the oblate ellipsoidal capsules and the small spherical capsules are placed with the initial configuration as shown in Fig. 10(a). After the pressure gradient is applied, the large capsules remain in the center of the channel, whereas the small capsules move toward the boundary wall (See Fig. 10(b)). In general, the DDS particle is assumed smaller than the red blood cells. Then, the DDS particle moves toward the wall of the blood vessel, which makes it easy to reach the inflammation or a diseased part through the cleft of the blood vessel.

4. Summary
A simulation of the Front-Tracking method was presented in this paper. The motion of the droplet under the gravity field and the shear flow were shown. Lateral migration of elastic capsules was examined. The elastic capsules of the same size moved to the center of the Poiseuille flow. In the mixture of the small and large capsules, the large capsules moved to the center, whereas the small capsules moved toward the boundary walls. In this study, we showed the simulation method to obtain the fundamental information to design the DDS particle and biological cells.
Figure 8. Center of the capsule $y/a$ starting from different initial positions as a function of time $t p_x a / \mu$. The dashed line indicates the center of the channel.

Figure 9. Hydrodynamic conductance $\nu/\nu_0$ of the channel as a function of $t p_x a / \mu$.

Figure 10. Small capsules move toward the wall of the channel, whereas large ones remain near the center of the channel.
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References
[1] Barthès-Biesel D, Yamaguchi T, Ishikawa T and Lac E 2006 From passive motion of capsules to active motion of cells J. Biomech. Sci. and Engin.
[2] Pozrikidis C 2003 Modeling and Simulation of Capsules and Biological Cells (New York:Chapman & Hall/CRC)
[3] Pozrikidis C 2010 Computational Hydrodynamics of Capsules and Biological Cells (New York:Chapman & Hall/CRC)
[4] Makino M and Sano O Motion of droplets under shear flow with suction Fluid Dyn. Res. (accepted for publication)
[5] Peskin C S 1977 Numerical analysis of blood flow in the heart J. Comput. Phys. 25 220
[6] Peskin C S and McQueen D.M 1989 A three-dimensional computational method for blood flow in the heart I. Immersed elastic fibers in a viscous in compressible fluid J. Comput. Phys. 81 372
[7] Peskin C S and Printz B.F 1993 Improved volume conservation in the computation of flows with immersed boundaries J. Comput. Phys. 105 33
[8] Peskin C S 2002 The immersed boundary method Acta Numer. 11 479
[9] Tryggvason G, Scardovelli R and Zaleski S 2011 Direct numerical simulations of gas-liquid multiphase flows (New York:Cambridge University Press)
[10] Bunner B and Tryggavason G 2002 Dynamics of homogeneous bubbly flows Part 1. Rise velocity and microstructure of the bubbles J. Fluid. Mech. 466 17
[11] Bunner B and Tryggavason G 2002 Dynamics of homogeneous bubbly flows Part 2. Velocity fluctuations J. Fluid. Mech. 466 53
[12] Bunner B and Tryggavason G 2003 Effect of bubble deformation on the properties of bubbly flows J. Fluid. Mech. 495 77
[13] Esmaeeli A and Tryggavason G 1998 Direct numerical simulations of bubbly flows. Part 1. Low Reynolds number arrays J. Fluid. Mech. 377 313
[14] Esmaeeli A and Tryggavason G 1999 Direct numerical simulations of bubbly flows. Part 2. Moderate Reynolds number arrays J. Fluid. Mech. 385 325
[15] Esmaeeli A and Tryggavason G 2005 A direct numerical simulation study of the buoyant rise of bubbles at O(100) Reynolds number Phys. Fluids 17 093303
[16] Lu J and Tryggavason G 2006 Numerical study of turbulent bubbly downflows in a vertical channel Phys. Fluids 18 103302
[17] Lu J and Tryggavason G 2008 Effect of bubble deformability in turbulent bubbly upflow in vertical channel Phys. Fluids 20 040701
[18] Brackbill J U and Ruppel H M 1986 FLIP: a method for adaptively zoned, particle-in-cell calculations in two dimensions J. Comput. Phys. 65 314
[19] Charrier J, Shrivastava S and Wu R 1989 Free and constrained inflation of elastic membranes in relation to thermoforming-non-axisymmetric problems J. Strain. Analysis 24 55
[20] Zinchenko A, Rother M and Davis R 1997 A novel boundary-integral algorithm for viscous interaction of deformable drops Phys. Fluids 9 1493