



An immersed boundary method for simulating vesicle dynamics in three dimensions



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ABSTRACT

We extend our previous immersed boundary (IB) method for 3D axisymmetric inextensible vesicle in Navier–Stokes flows (Hu et al., 2014 [17]) to general three dimensions. Despite a similar spirit in numerical algorithms to the axisymmetric case, the fully 3D numerical implementation is much more complicated and is far from straightforward. A vesicle membrane surface is known to be incompressible and exhibits bending resistance. As in 3D axisymmetric case, instead of keeping the vesicle locally incompressible, we adopt a modified elastic tension energy to make the vesicle surface patch nearly incompressible so that solving the unknown tension (Lagrange multiplier for the incompressible constraint) can be avoided. Nevertheless, the new elastic force derived from the modified tension energy has exactly the same mathematical form as the original one except the different definitions of tension. The vesicle surface is discretized on a triangular mesh where the elastic tension and bending force are calculated on each vertex (Lagrangian marker in the IB method) of the triangulation. A series of numerical tests on the present scheme are conducted to illustrate the robustness and applicability of the method. We perform the convergence study for the immersed boundary forces and the fluid velocity field. We then study the vesicle dynamics in various flows such as quiescent, simple shear, and gravitational flows. Our numerical results show good agreements with those obtained in previous theoretical, experimental and numerical studies.

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1. Introduction

A vesicle is a liquid droplet with a radius of about 10 μm enclosed by a phospholipid membrane suspended in an incompressible viscous fluid media. Such phospholipid membrane consists of two-layer tightly packed lipid molecules with hydrophilic heads facing the exterior and interior fluids while the hydrophobic tails hide in the middle. This bilayer membrane has the thickness about 6 nm and exhibits resistance against membrane dilation and bending. Therefore, it is quite natural to regard this membrane as an incompressible surface with mechanical functions determined by some energy functional [16]. Thus, the dynamics of vesicle in fluids can be determined by the membrane incompressibility, bending, and hydrodynamical forces. The study of vesicle dynamics in fluid flow has become an active research area in the communities

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of soft matter physics and computational fluid mechanics in the past years. For example, understanding of vesicle behaviors in fluid flows might lead to a better knowledge of red blood cells (RBCs) in blood simply because they both share similar mechanical behaviors [33]. Certainly, it has other practical applications such as a drug-delivery vehicle for cancer therapy [40] and a micro-reactor [13] for enzymatic mRNA synthesis in bioengineering.

The interaction between the vesicle and surrounding fluid makes the dynamics rich from physical point of view. For instance, a vesicle can undergo tank-treading, tumbling, or trembling motion under shear flow, see [6] and the references therein. For the past two decades, the vesicle dynamics in general flows (particularly in shear flow) have been extensively studied by experiments [22,24,6], theories [25,32,28,11], and numerical simulations, see the detailed references below.

The numerical simulations of the vesicle problem not only involve a two-phase incompressible flow but also require to enforce an incompressibility constraint of the membrane surface, which makes the problem more challenging. The numerical methods for simulating vesicle problems in literature can be characterized by how the membrane surface is represented and how the fluid equations are solved. Based on this characterization, several methods have been developed such as boundary integral method [26,43,44,3,45,50,12], level set method [29,37,27,30,8], phase field method [9,2,30,1], particle collision method [34], immersed interface method [21,41], and immersed boundary method or front-tracking method [18,20,48,17]; just to name a few recent ones. In all of these numerical methods, how to impose the membrane incompressibility constraint is an important issue. The surface tension in vesicle problems, which has a different physical meaning from that in general two-phase flow problems, is unknown a priori and in fact acts like Lagrange multiplier to enforce the local incompressibility along the surface. This is exactly the same role played by the pressure to enforce the fluid incompressibility in Navier–Stokes equations.

There are two different approaches to enforce the local incompressibility constraint in literature. The first one needs to discretize the whole equations first (regardless of using boundary integral, finite element, or finite difference method) and then to solve the discretized equations simultaneously for the tension and fluid variables. This approach can be explicit or semi-implicit depending on how we treat the tension force computations. There usually exists a trade-off between the time-step stability and efficiency in those algorithms simply because iterative procedures are needed. Most of the boundary integral method [45,3,50] or level set method [37,27] fall into this category. Another approach, which was used in our previous 3D axisymmetric case [17], is called a penalty idea. Instead of keeping the vesicle membrane locally incompressible, the penalty idea makes the vesicle surface patch nearly incompressible by introducing a modified elastic tension energy. This approach replaces the unknown tension by a spring-like tension depending on the surface configuration so that we can avoid solving the whole system to obtain the variable tension, which significantly simplifies the numerical algorithm. In this paper, we extend our previous immersed boundary (IB) method for simulating incompressible vesicles in 3D axisymmetric Navier–Stokes flows [17] to general three dimensions. We shall show that the new elastic force derived from the modified tension energy has exactly the same mathematical form as the original elastic force except for the different definitions of the tension. We validate this approach by performing several numerical tests in our simulations.

The rest of the paper are organized as follows. In Section 2, we present the governing equations for the vesicle problem under the immersed boundary formulation. We also provide some notions in classical differential geometry that will be used to compute the geometrical quantities of the vesicle surface mathematically and numerically. Then we introduce our approach for a nearly incompressible vesicle surface and the modified energy. The detailed numerical algorithm is described in Section 3; we first explain how to evaluate the mean curvature vector and bending force terms on a triangulated surface, then outline the complete time-stepping scheme for the algorithm, and finally discuss how to maintain the surface mesh quality during the simulations. A series of numerical tests to validate our present algorithm is given in Section 4 which is followed by conclusion and future work in Section 5.

2. Equations of motion

We consider a single incompressible vesicle $\Gamma(t)$ suspended in a three-dimensional domain Ω filled with viscous incompressible Navier–Stokes fluid. For the IB formulation in which the fluid-related quantities are represented in Eulerian manner while the vesicle-related ones are in Lagrangian manner, the governing equations can be written as follows.

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f} \quad \text{in } \Omega, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega, \quad (2)$$

$$\mathbf{f}(\mathbf{x}, t) = \int_{\Gamma} \mathbf{F}(r, s, t) \delta(\mathbf{x} - \mathbf{X}(r, s, t)) dA, \quad (3)$$

$$\frac{\partial \mathbf{X}}{\partial t}(r, s, t) = \mathbf{U}(r, s, t) = \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(r, s, t)) d\mathbf{x}, \quad (4)$$

$$\nabla_s \cdot \mathbf{U} = 0 \quad \text{on } \Gamma. \quad (5)$$

Here, we assume that the fluids inside and outside vesicle have the same density ρ and viscosity μ . Eqs. (1) and (2) are the incompressible Navier–Stokes equations with the fluid velocity $\mathbf{u}(\mathbf{x}, t)$ and the pressure $p(\mathbf{x}, t)$, where $\mathbf{x} = (x, y, z)$ is

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