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Diffuse interface models of locally inextensible vesicles in a viscous fluid

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ABSTRACT

We present a new diffuse interface model for the dynamics of inextensible vesicles in a viscous fluid with inertial forces. A new feature of this work is the implementation of the local inextensibility condition in the diffuse interface context. Local inextensibility is enforced by using a local Lagrange multiplier, which provides the necessary tension force at the interface. We introduce a new equation for the local Lagrange multiplier whose solution essentially provides a harmonic extension of the multiplier off the interface while maintaining the local inextensibility constraint near the interface. We also develop a local relaxation scheme that dynamically corrects local stretching/compression errors thereby preventing their accumulation. Asymptotic analysis is presented that shows that our new system converges to a relaxed version of the inextensible sharp interface model. This is also verified numerically. To solve the equations, we use an adaptive finite element method with implicit coupling between the Navier–Stokes and the diffuse interface inextensibility equations. Numerical simulations of a single vesicle in a shear flow at different Reynolds numbers demonstrate that errors in enforcing local inextensibility may accumulate and lead to large differences in the dynamics in the tumbling regime and smaller differences in the inclination angle of vesicles in the tank-treading regime. The local relaxation algorithm is shown to prevent the accumulation of stretching and compression errors very effectively. Simulations of two vesicles in an extensional flow show that local inextensibility plays an important role when vesicles are in close proximity by inhibiting fluid drainage in the near contact region.

1. Introduction

Vesicles are fluid-filled sacs bounded by a closed lipid bilayer membrane. Vesicles play a critical role in intracellular transport of molecules and proteins [4]. Vesicles have been used as drug delivery vehicles [56], microreactors [21] and as models of more complex biostructures such as red blood cells (RBCs) [55]. RBCs and vesicles are known to undergo complex motions and shape changes under applied flows (e.g., see [2,10,15,22,28,38,50]) and transitions from stationary shapes (tank-treading) to trembling to tumbling have been observed as a function of flow conditions and membrane characteristics. RBCs resist shear deformation due to the presence of a membrane cytoskeleton and also resist bending and area dilatation (e.g., see [3,50,65]), while the lipid bilayer membranes in vesicles are liquid-like, resist bending and are largely inextensible

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(e.g., see [39,55]). In this paper, we focus on the dynamics of homogeneous vesicles, although our results apply more generally to the case in which there may be several lipid components on the membrane that can induce the formation of rafts.

Most experimental results on vesicles are performed in the low Reynolds number regime, see e.g. [15,28,42]. Under these conditions inertial effects can be neglected and the Stokes limit considered, which allows the development of small-deformation perturbation theories [13,29,36,45–47,64], which all qualitatively predict the experimentally observed tank-treading and tumbling motion. Various numerical approaches have also been considered in the Stokes limit to analyze tank-treading and tumbling, e.g. [6,8,7,24,30,31,33,48,51,57,60,61,66]. Except for [30] in which the vesicle shape was assumed to be a fixed ellipsoid, all other models are of Helfrich type and consider a membrane free energy

$$\mathcal{E} = \int_\Gamma \frac{1}{2} b_N (H - H_0)^2 \, d\Gamma + \int_\Gamma b_G K \, d\Gamma \tag{1}$$

with membrane $\Gamma(t)$, total curvature H, spontaneous curvature H_0, normal bending rigidity b_N, Gaussian bending rigidity b_G and Gaussian curvature K. We focus on the case in which the vesicle is homogeneous and its topology does not change. Then b_N, H_0 and b_G may be assumed to be constant and the Gaussian bending energy only contributes a constant and can therefore be neglected. Lagrange multipliers are used to enforce the inextensibility constraint, which can be considered as a global constraint to enforce a constant area of the membrane, but allowing for local variations, or as a stronger local constraint. The jump condition for the fluid stress tensor $\mathbf{S} = -p\mathbf{I} + \nu\mathbf{D}$, where p is the pressure, ν is the viscosity, and $\mathbf{D}$ is twice the rate of deformation tensor $\mathbf{D} = \nabla\mathbf{v} + (\nabla\mathbf{v})^T$, with velocity $\mathbf{v}$, along the membrane then reads

$$[\mathbf{S}\cdot\mathbf{n}]_\Gamma = \frac{\delta\mathcal{E}}{\delta\Gamma} \quad \text{unconstrained,} \tag{2}$$

$$[\mathbf{S}\cdot\mathbf{n}]_\Gamma = \frac{\delta\mathcal{E}}{\delta\Gamma} + \lambda_{\text{global}} H\mathbf{n} \quad \text{global area constraint,} \tag{3}$$

$$[\mathbf{S}\cdot\mathbf{n}]_\Gamma = \frac{\delta\mathcal{E}}{\delta\Gamma} + \lambda_{\text{local}} H\mathbf{n} + \nabla_\Gamma \lambda_{\text{local}} \quad \text{local inextensibility constraint,} \tag{4}$$

where $[f]_\Gamma = f_{\text{outer}} - f_{\text{inner}}$, $\mathbf{n}$ is the normal pointing out of the vesicle, and ∇_Γ is the surface gradient $\nabla_\Gamma = \mathbf{P}\nabla$, with the projection operator $\mathbf{P} = \mathbf{I} - \mathbf{n}\otimes\mathbf{n}$. The Lagrange multipliers are functionals of the fluid velocity $\mathbf{v}$ and are obtained by requiring

$$\frac{d}{dt}\int_\Gamma d\Gamma = \int_\Gamma H\mathbf{v}\cdot\mathbf{n}\, d\Gamma = 0, \quad \text{global area constraint,}$$

$$\nabla_\Gamma \cdot \mathbf{v} = 0, \quad \text{local inextensibility constraint.}$$

We remark that locally inextensible vesicles also conserve the global surface area. The jump condition for the velocity in all cases is

$$[\mathbf{v}]_\Gamma = 0.$$

Due to the linearity of the Stokes problem, efficient algorithms can be derived to solve the coupled fluid-structure flow problem, e.g. [7,57,60,61,66]. When inertial forces are considered, the development of efficient algorithms remains a significant challenge.

Inertial effects can become important in a variety of biophysical applications. Flowing vesicles/RBCs in larger blood vessels such as arterioles and arteries may experience Reynolds numbers of order unity or higher, especially if the vessels are constricted due to diseases such as thrombosis, e.g. [5,62]. Large Reynolds numbers may also be found in biomedical devices such as ventricular assist devices, e.g., [23]. Motivated by these applications inertial effects are considered in [16,32,34,41,43,54], which found that the classical tumbling behavior of highly viscous vesicles is no longer observed at moderate Reynolds numbers.

The Navier–Stokes equations inside and outside the vesicle read

$$\rho(\partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) - \nabla\cdot\mathbf{S} = 0 \tag{5}$$

$$\nabla\cdot\mathbf{v} = 0 \tag{6}$$

with density $\rho = \rho_{1,2}$ and stress tensor $\mathbf{S} = \mathbf{S}_{1,2} = -p\mathbf{I} + \nu_{1,2}\mathbf{D}$. Here, the notation $\rho_{1,2}$ means ρ_1 inside and ρ_2 outside the vesicle. The global area constraint, which can be treated explicitly, has been used by [9] within a front tracking method, by [17,18,25,44] within phase field methods, and was also considered in [53] within a level-set approach.

The local inextensibility constraint is more delicate and leads to additional nonlinear coupling in the model. This has been considered within a level set approach in [16,34,53,54], immersed boundary methods [31,32] and phase field methods [8,7,34,43]. Capsule-like models have also been considered using strain-energy functions that penalize local stretching, e.g. [12,41].

In [53,54] the system is rewritten as a single-fluid model by considering the jump conditions for the fluid stress tensor as a body–force term with a delta-function δ_Γ to localize the force at the membrane. An iterative multi-step projection