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An adaptive meshfree method for phase-field models of biomembranes. Part II: A Lagrangian approach for membranes in viscous fluids

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ABSTRACT

We present a Lagrangian phase-field method to study the low Reynolds number dynamics of vesicles embedded in a viscous fluid. In contrast to previous approaches, where the field variables are the phase-field and the fluid velocity, here we exploit the fact that the phase-field tracks a material interface to reformulate the problem in terms of the Lagrangian motion of a background medium, containing both the biomembrane and the fluid. We discretize the equations in space with maximum-entropy approximants, carefully shown to perform well in phase-field models of biomembranes in a companion paper. The proposed formulation is variational, lending itself to implicit time-stepping algorithms based on minimization of a time-incremental energy, which are automatically nonlinearly stable. The proposed method deals with two of the major challenges in the numerical treatment of coupled fluid/phase-field models of biomembranes, namely the adaptivity of the grid to resolve the sharp features of the phase-field, and the stiffness of the equations, leading to very small time-steps. In our method, local refinement follows the features of the phase-field as both are advected by the Lagrangian motion, and large time-steps can be robustly chosen in the variational time-stepping algorithm, which also lends itself to time adaptivity. The method is presented in the axisymmetric setting, but it can be directly extended to 3D.

1. Introduction

Biomembranes self-assemble in a fluid, and often, the fluid mechanics are important in their dynamical behavior. Examples include the dynamics of vesicles in shear flows (see, e.g., [1–4]), or the relaxation dynamics of membrane structures brought out-of-equilibrium [5,6]. Describing explicitly the fluid surrounding biomembranes may also be useful in studying the interactions between membranes and other structures [7]. Here, we consider the simplest, yet very common and useful model of a biomembrane: an inextensible interface with curvature elasticity, given by the Helfrich energy. We ignore here the bilayer architecture, the monolayer extensibility, the surface viscosity, and the inter-monolayer friction, which can be important in some situations [8]. Our goal here is to develop a robust and efficient computational technique for biomembranes embedded in a viscous fluid, capable of handling arbitrarily large shape changes and the associated flows. We resort to phase-field models of biomembranes, and propose a non-conventional discretization of the membrane-fluid system. In a companion paper [9], we have shown that high-order phase-field models of biomembranes can be accurately approximated

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in a direct Galerkin approach with the maximum-entropy meshfree approximants [10], in an adaptive, accurate and efficient way. Here, we elaborate a Lagrangian method for the dynamics of vesicles embedded in a viscous fluid, which builds on the meshfree approximation of the phase-field equations. The proposed method shares common features with the optimal mass transport (OTM) method presented in [11].

1.1. Background

A number of models and numerical approaches have been proposed to analyze the hydrodynamics of fluid membranes in a viscous fluid. These include a mesoscopic model, combining a particle-based method for the fluid and a dynamically triangulated surface model for the membrane [3], which has been put forth to study the effect of membrane viscosity and thermal fluctuations in the dynamical behavior of vesicles in simple shear flow, as well as the behavior of vesicles and red blood cells in microcapillaries [12]. Other methods rely on conventional continuum mechanics models, e.g., [13,14], where a sharp-interface Helfrich model coupled with a Lagrangian form of the Navier–Stokes equations is discretized with finite elements. An alternative sharp-interface approach in three dimensions was presented in [15,4], which relies on spherical harmonics representations of the vesicle shapes and fields on it, and on a boundary integral method for the Stokes flow. This method has been exercised in systems containing many interacting vesicles. Immersed boundary methods [16] represent an alternative approach to handle fluid–structure interaction, maintaining the Eulerian framework for the fluid media and the Lagrangian description for solid objects immersed in the flow. This family of methods have been applied to understand the hydrodynamic effects on fluid vesicles and biomembranes in [17,18]. Phase-field models of vesicles [19] have also been coupled with the ambient hydrodynamics [20,21], through an Eulerian description of the fluid with a source term of membrane elastic forces, and a transport equation to advect the phase-field representing the membrane. Alternative phase-field approaches to vesicles in a flow have been proposed in [22,23], where the local area inextensibility was also accounted for, and in [24].

Phase-field models offer advantages when compared to sharp-interface models, in that they provide unified treatment of interface tracking and surface mechanics with a single partial differential equation (PDE) governing the phase-field. Phase-field approaches do not suffer from severe mesh distortions, and can easily deal with large deformations and even topology changes [22,25] without demanding specific reparametrization techniques [13] or control of the tangential motions of the nodes [26]. In contrast, phase-field models are encoded by nonlinear PDEs, often high-order, which develop sharp features, and therefore present computational challenges. In phase-field models of biomembranes, an artificial length-scale ϵ governing the width of the smeared interface is introduced, and the sharp-interface limit is recovered as $\epsilon \to 0$ [19,22,27]. For phase-field models to accurately represent the sharp-interface limit, ϵ needs to be much smaller than other relevant dimensions in the problem. Furthermore, this length-scale needs to be resolved by the computational grids, typically leading to expensive calculations. From a practical viewpoint, the high computational cost, associated with increasing the dimension of the problem and having to resolve numerically the (small) thickness of the smeared interface, can be outweighed by their simplicity, making them amenable to scalable parallel implementations. Besides, the computational cost can be considerably mitigated with spacial adaptivity [28,29].

1.2. The proposed method

In previous phase-field approaches to the ambient hydrodynamics-biomembrane mechanics, the problem is formulated in an Eulerian frame, as a coupled system combining the fluid flow equations with a source term coming from curvature elasticity forces and the advection of the phase-field with the flow, in which the phase-field and the fluid velocity (and pressure) are the unknowns [22,25]. In such approaches, adaptive strategies, not proposed so far, would require cumbersome grid projection steps. Since in the present situation the phase-field tracks a material interface, here we view the phase-field as a material property, and formulate a Lagrangian description of the problem in which the unknown is the Lagrangian motion of the background medium, containing both the fluid and the smeared interface (see Fig. 1 for an illustration). See [30] for a related approach. We particularize the model with the phase-field approach proposed by Du et al. [19], and since biomembranes often operate in the limit of vanishing Reynolds number, describe the hydrodynamics with Stokes equations.

With the Lagrangian viewpoint, when discretized in space, the coupled membrane-fluid model becomes a nonlinear dissipative particle system, driven by curvature elasticity and dragged by a viscous force admitting a dissipation potential, whose dynamics minimize an action [31] subject to area and volume constraints. With the same spirit as variational integrators for Hamiltonian systems [32], we choose to discretize in time the action, and then derive by constrained minimization the discrete evolution equations from it, rather than discretizing in time the continuous evolution equations. The method results in time-incremental nonlinear minimization problems, as in modern treatments of dissipative processes in materials science following the seminal work in [33]. As a consequence, it is possible to overcome the stiffness of the dynamics (given by the fourth-order nature of the PDE) and take robustly large time-steps. Furthermore, the algorithm is automatically nonlinearly stable as the energy monotonically decreases.

If the initial grid adapts to the features of the phase-field, adaptivity is advected by the Lagrangian map, and therefore local refinement along the dynamics is accomplished for free (see Fig. 1). The Lagrangian framework allows us to pull-back the successive states of the system to a reference configuration. Thus, we avoid the calculation of the meshfree basis functions in every step of the evolution. It has been shown that the meshfree method considered here can withstand significant