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An adaptive meshfree method for phase-field models of biomembranes. Part I: Approximation with maximum-entropy basis functions

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ABSTRACT

We present an adaptive meshfree method to approximate phase-field models of biomembranes. In such models, the Helfrich curvature elastic energy, the surface area, and the enclosed volume of a vesicle are written as functionals of a continuous phase-field, which describes the interface in a smeared manner. Such functionals involve up to second-order spatial derivatives of the phase-field, leading to fourth-order Euler–Lagrange partial differential equations (PDE). The solutions develop sharp internal layers in the vicinity of the putative interface, and are nearly constant elsewhere. Thanks to the smoothness of the local maximum-entropy (*max-ent*) meshfree basis functions, we approximate numerically this high-order phase-field model with a direct Ritz–Galerkin method. The flexibility of the meshfree method allows us to easily adapt the grid to resolve the sharp features of the solutions. Thus, the proposed approach is more efficient than common tensor product methods (e.g. finite differences or spectral methods), and simpler than unstructured C^0 finite element methods, applicable by reformulating the model as a system of second-order PDE. The proposed method, implemented here under the assumption of axisymmetry, allows us to show numerical evidence of convergence of the phase-field solutions to the sharp interface limit as the regularization parameter approaches zero. In a companion paper, we present a Lagrangian method based on the approximants analyzed here to study the dynamics of vesicles embedded in a viscous fluid.

1. Introduction

Biomembranes are the fundamental separation structure in animal cells, and are responsible for the compartmentalization of the cell or for the transport of substances through cargo vesicles or tubes. They also play a key role in bio-mimetic engineered systems [1]. Their complex behaviour, rich physical properties, formation and dynamics have been objects of experimental and theoretical investigation for biologists, chemists and physicists during many years [2,3]. Biomembranes are composed by several kinds of lipids self-assembled in a fluid bilayer, which presents a liquid behaviour in-plane and solid out-of-plane [4]. Vesicles are closed biomembranes, which play an important role in biophysical processes such as in the delivery of proteins, antibodies or drugs into cells, and separation of different types of biological macromolecules within cells. Vesicles serve as simplified models of more complex biological systems, and can be used to study the interaction between lipid bilayers and the surrounding medium, e.g. under osmotic stress [5], shear flow [6], or electrical fields [7].

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Depending on the lipid composition, lipid bilayers can phase-separate forming multicomponent vesicles [8], which have also been the object of numerous studies as model systems for rafts.

Lipid bilayers can be modeled by very different techniques, depending on the focus. Atomistic [9] and coarse-grained [10] molecular dynamics (MD) can access molecular processes and the self-assembly. However, due to the slow relaxation of the bending modes, the computational cost of molecular simulations scales as L^6, where L is the lateral dimension of the system [11]. Even if coarse-grained MD simulations have been able to describe the collective dynamics of membrane patches of tens of nanometers, this sets a very stringent limit on the system sizes accessible with these methods. Other mesoscopic methods such as dynamically triangulated surfaces have been proposed to deal with intermediate scales [12]. On the other end of the spectrum, continuum mechanics has shown great success over the last decades in describing the equilibrium shapes of vesicles [4,13,14]. Continuum models have also helped understand the dynamics of fluctuations of bilayers [15], or the shape dynamics of membranes [16,17]. Continuum mechanics models of biomembranes disregard atomic details, but still can incorporate many important effects such as the bilayer asymmetry, the spontaneous curvature, the diffusion of chemical species on the bilayer, or the dissipative mechanisms arising from the friction between the lipids [18]. Furthermore, these methods can easily access wide spans of time and length scales. The main drawback of these models is that they are usually formulated as complex nonlinear high-order partial differential equations (PDE). Here, we focus on the numerical approximation of a simple curvature model for biomembranes.

The Canham–Helfrich functional [19,20] is a widely accepted continuum model for the curvature elasticity of fluid membranes, which explains to a large extent the observed morphologies of vesicles. This sharp interface model has been the basis of a number of numerical parametric approaches for the equilibrium analysis of axisymmetric and three-dimensional vesicles. The resulting equations for the parameterization are fourth-order nonlinear PDE. This functional is reparameterization invariant, which reflects mathematically the in-plane fluidity of lipid bilayers above the transition temperature. This feature poses numerical difficulties to parametric methods, since this invariance needs to be controlled to avoid serious mesh distortions [21,22].

Phase-field counterparts of this model have been proposed and exercised numerically [23–25]. Although these methods increase the dimension of the problem, they naturally overcome the limitations of parametric methods when extreme shape, or even topology changes are present, and produce more robust simulations. Furthermore, these methods are more amenable to scalable parallel computations for complex systems, particularly when coupling them to the fluid mechanics of the ambient medium. Yet, the numerical solution of these models, again expressed mathematically as a nonlinear fourth-order PDE, is challenging. Here, we propose to address the high-order character of the equations and the sharp fronts they develop with an adaptive meshfree method. We also establish the ability of the local maximum-entropy approximants [26] to accurately and efficiently approximate equilibrium solutions of the phase-field model with a straight Ritz–Galerkin approach. In a companion paper [27], we propose a Lagrangian method to deal with the dynamics of vesicles embedded in a viscous fluid in the low Reynolds number limit, representative of most biological situations of interest.

The outline of the paper is as follows. Section 2 introduces the sharp interface and the phase-field models for the curvature elasticity of biomembranes, as well as a brief account of the numerical strategies to address these models. Section 3 describes the discretization of the phase-field functionals with the local maximum-entropy approximations schemes, the algorithm to find equilibrium solutions, and the method used to distribute the nodes. Numerical experiments to evaluate the performance of the approximants and the adaptive strategy are presented in Section 4. The final conclusions are collected in Section 5.

2. Sharp interface model, phase-field model, and its numerical treatment

2.1. Sharp interface model

In the sharp interface (S-I) approach, the membrane is a mathematical surface without thickness. The equilibrium shapes of vesicles minimize the Canham–Helfrich energy under area and enclosed volume constraints follow from

$$\begin{aligned} \text{(S-I model) Minimize} \quad & E(\Gamma) = \frac{k}{2}\int_\Gamma (H - C_0)^2 dS + k_G \int_\Gamma K dS \\ \text{subject to} \quad & V(\Gamma) = \frac{1}{3}\int_\Gamma \boldsymbol{x}\cdot\mathbf{n} dS = V_0 \\ & A(\Gamma) = \int_\Gamma dS = A_0, \end{aligned}$$

where Γ is the surface, k the bending rigidity, k_G the Gaussian bending rigidity, H the mean curvature, K the Gaussian curvature, $\mathbf{n}$ the normal to the surface, V_0 and A_0 are the prescribed volume and surface area, and C_0 is the spontaneous curvature. For surfaces of constant topology, the second integral in the curvature energy is a constant, and for this reason it is often ignored. We do not consider this term in the remainder of the paper, although is can be easily incorporated.

The area constraint comes from the near inextensibility of lipid bilayers under the usual applied forces. The volume can be regulated by osmotic effects, since biomembranes are semi-permeable. If the volume V_0 is smaller than the volume enclosed