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Parametric FEM for geometric biomembranes

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ABSTRACT

We consider geometric biomembranes governed by an L^2-gradient flow for bending energy subject to area and volume constraints (Helfrich model). We give a concise derivation of a novel vector formulation, based on shape differential calculus, and corresponding discretization via parametric FEM using quadratic isoparametric elements and a semi-implicit Euler method. We document the performance of the new parametric FEM with a number of simulations leading to dumbbell, red blood cell and toroidal equilibrium shapes while exhibiting large deformations.

1. Introduction

Lipids consist of a hydrophilic head group and one or more hydrophobic hydrocarbon tails. When lipid molecules are immersed in aqueous environment at a proper concentration and temperature they spontaneously aggregate into a bilayer or membrane that forms an encapsulating bag called vesicle. This phenomenon is of interest in biology and biophysics because lipid membranes are ubiquitous in biological systems, and an understanding of vesicles provides an important element to understand real cells. Canhan and Helfrich [1,2] were the first to introduce over 35 years ago, a model for the equilibrium shape of vesicles consisting of minimization of the *bending elasticity* or curvature energy. The structure of lipid membranes is that of a two dimensional, oriented, incompressible and viscous fluid. Phenomenological [1,2] and rigorous continuum mechanical [3–5] approaches agree that the membrane Γ is endowed with a bending or elastic energy. The simplest form of this energy is

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$$\kappa \int_\Gamma h^2 + \kappa_G \int_\Gamma k,$$

where h and k are the mean and Gauss curvature, respectively; and κ and κ_G are the constant bending coefficients. For closed surfaces without topological changes, the Gauss–Bonnet theorem [6, Section 8.5] yields the equivalence (up to scaling) between the above energy and the "Willmore" energy [7] defined by

$$W(\Gamma) := \frac{1}{2} \int_\Gamma h^2. \tag{1}$$

If the temperature and osmotic pressure of the vesicle do not change, the enclosed volume and surface area can be assumed to be conserved. The former is a consequence of the impermeability of the membrane. The latter is because the number of molecules remains fixed in each layer and the energetic cost of stretching or compressing the membrane is much larger than the cost of bending deformations. Refer to [8–10] for more details.

In this work, we consider the Willmore energy model (1) with isoperimetric area and volume constraints. The combined effect of the bending elasticity with the surface and volume constraints generates a great variety of non-spherical shapes, in contrast to the characteristic spherical equilibrium shapes of simple liquids which are governed by isotropic surface tension. Describing the membrane by quantities all defined on the surface (energy, area and volume), equilibrium shapes are obtained as stationary states of a geometric evolution equation. For other aspects more related to the dynamics, the effect of the surrounding fluid should be taken into account. We study this effect in [11] and compare it with the geometric model.

Formally, the geometric model is a gradient flow for a suitable shape functional $J(\Gamma)$: find the evolution of the surface $\Gamma = \Gamma(t)$ such that its velocity $\boldsymbol{v}$ is given by

$$\langle \boldsymbol{v}, \boldsymbol{w} \rangle = -dJ(\Gamma; \boldsymbol{w}) \quad \forall \boldsymbol{w}, \tag{2}$$

where $dJ(\Gamma; \boldsymbol{w})$ is the shape derivative of $J(\Gamma)$ in the direction of $\boldsymbol{w}$ and $\langle \cdot, \cdot \rangle$ is a scalar product determining the type of flow [12].

The shape derivative of the Willmore energy (1) in three dimensions is given by

$$dW(\Gamma; \boldsymbol{w}) = \int_\Gamma \left(-\Delta_\Gamma h - \frac{1}{2} h^3 + 2kh\right) w, \tag{3}$$

where $w = \boldsymbol{\nu} \cdot \boldsymbol{w}$ is the normal component of $\boldsymbol{w}$. The L^2-gradient flow (i.e. $\langle \boldsymbol{v}, \boldsymbol{w} \rangle := \int_\Gamma \boldsymbol{v} \cdot \boldsymbol{w}$) obtained from (2) with $J = W$, namely using (3), is known as the Willmore flow and is a highly nonlinear 4th order geometric partial differential equation (PDE) on $\Gamma(t)$. We refer to [13] for a general discussion of discrete gradient flows.

Parametric finite element methods (FEM) have already been proposed for the Willmore flow without constraints [14,15] and with constraints [16]. A chief difficulty is to make sense of Gauss curvature k within a variational framework. The scheme of Rusu [15] is the first of this class for (1) without constraints. That of Dziuk [14] copes with undesirable tangential motions observed in Rusu's scheme near equilibrium and presents a stability estimate for special initial conditions. In both cases, the formulation involves vector quantities (position and curvature). In contrast, Garcke et al. [16] present a scalar scheme for (1) with constraints and evolve the interface in the direction of an averaged normal. The latter is somewhat related to the method of Bänsch et al for surface diffusion [17]. All these schemes are implemented with piecewise linear elements and exhibit difficulties to start; they are due to geometric inconsistency, a new concept that we discuss briefly in Section 4.4 and fully in [18]. Alternative techniques are also available in the literature, for instance the phase field approach [19,20], threshold dynamics [21] and level set method [22]. An advantage of our parametric method over the alternatives is the capability to easily increase the approximation order of the interface. In addition, quadratics are more robust than linears regarding mesh quality; this adds to several other important features for fourth order problems discussed in Section 4.5. Finally note that the number of degrees of freedom associated with the parametric approach is that of a 2D problem, whereas for the phase field or level set methods a full 3D problem is to be solved, perhaps with the help of adaptive meshes or narrow band methods to improve efficiency. These advantages are at the expense of difficulties in executing topological changes, especially in 3D.

In this paper, we give a rather concise derivation of a novel vector formulation for (1) with constraints that hinges on shape differential calculus [23,12]. In fact, we derive the following vector form of the shape derivative (Theorem 3.1)

$$dW(\Gamma; \boldsymbol{\phi}) = \int_\Gamma \nabla_\Gamma \boldsymbol{\phi} \cdot \nabla_\Gamma \mathsf{h} - \int_\Gamma (\nabla_\Gamma \mathsf{x} + \nabla_\Gamma \mathsf{x}^{\mathsf{T}}) \nabla_\Gamma \boldsymbol{\phi} : \nabla_\Gamma \mathsf{h} + \frac{1}{2} \int_\Gamma \mathrm{div}_\Gamma \mathsf{h}\, \mathrm{div}_\Gamma \boldsymbol{\phi}, \tag{4}$$

where $\boldsymbol{x}$ is the variable of integration or, with a slight abuse of notation, is also the identity over Γ. Since (4) is variational, it is the basis of a new parametric FEM with C^0-elements. We prefer quadratic isoparametric elements to linear elements, and discuss the reasons in Section 4.5. We evolve the computational domain at each time step via a semi-implicit Euler method; this is similar to [17,16,11,24,25,13,26,14] and is discussed in Section 4.1.

The contributions of this paper are as follows:

- We derive the novel variational formulation (4) and corresponding parametric FEM. The derivation, being based on concepts from shape differential calculus, is rather concise.