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A finite element method for viscous membranes

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ABSTRACT

The simulation of biological interfaces at the Living Cell scale relies on membrane models that are a combination of a finite–strain elastic part, typically modeling the contribution of a cytoskeleton, and a viscous part that models the contribution of the lipidic bilayer. The motion of these membranes is driven by a shape-dependent energy, modeled by means of the Canham–Helfrich formula or variants thereof. In this article we review the finite element formulation of elastic membranes, and then extend it so as to deal with the viscous behavior of lipidic bilayers. The resulting numerical method, which is easily implemented on codes developed for solid membranes, is assessed on the simulation of dynamical prolate-to-oblate transitions of simplified red blood cells under tweezing.

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1. Introduction

Fluidic behavior is characterized by the impossibility of rest under shear. Both in Nature and in biomedical applications there exist highly-deformable membranes that exhibit fluidic behavior. The most important example is that of lipidic bilayers, which are a basic constituent of the living cell membrane. They consist of two molecular layers of amphiphilic phospholipids, each layer exposing the hydrophilic ends of their molecules to the adjacent water and thus also keeping the hydrophobic ends away from it. The molecules in lipidic membranes exhibit very high tangential mobility, with relatively low layer-to-layer transfer rate. Molecular simulations have greatly improved the understanding of these systems, in particular of their tangential behavior [43,50,16,38]. However, for simulations at the scale of a whole Living Cell to be computable during biologically significant time lapses, continuum models are mandatory. The best candidate model corresponds to a two-dimensional fluid, flowing on a time-dependent, curved surface in three-dimensional space.

The actual rheological behavior of lipidic bilayers is predominantly viscous (i.e., Newtonian) and area-preserving [47,32,34], with a surface viscosity μ of about 5–13 $\times 10^{-9}$ Pa s m [55] that can take higher values, up to 2×10^{-6} Pa s m. Though some visco-elasticity may exist, recent rheometrical data suggest that it is not significant [21,22].

In this work we propose a method for the finite element simulation of viscous membranes. It is strongly based on variational methods that are well established in the field of Solid Mechanics, obtaining the discrete equations by perturbations of the appropriate energy. The presentation begins with a brief review of the finite element treatment of *elastic* membranes, for which details can be found in [24] and biological applications in [41,27,52,30,28]. In a suitable limit, the elastic operator tends to the viscous operator, to which the zero-tangential-divergence (inextensibility) condition is added to arrive at a realistic approximation of the surface fluidic behavior. The inextensibility condition introduces a Lagrange multiplier field P which plays the role of a non-homogeneous surface tension. A stabilization term proportional to the surface Laplacian of P is added to allow for the use of the same interpolants for all fields. As driving force for the motion, the Canham–Helfrich model [11,23] is added in order to study shape evolutions typical of biological membranes. Overall, the method seems to be the first to compute truly viscous and inextensible relaxation of membranes in general 3D geometries. This is illustrated by simulating the dynamical response of a (simplified) red blood cell under oscillatory tweezing.

Possible applications of the proposed method are numerous, such as dynamical studies of membrane adhesion [15], conformation [32], stomatocyte–discocyte–echinocyte [31] and other shape transformations [48,39], among many others.

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2. Elastic membranes

2.1. Membrane kinematics

The large–deformation kinematics of membranes is already well known but will be reviewed here as a basis for the extensions made later on. The interested reader is referred, for example, to the detailed articles by Holzapfel et al. [24] and Bonet et al. [6].

Consider an open set $\hat{T}$ in $\mathbb{R}^2$, which will typically be a master finite element. The material points of some part of the membrane are associated to $\hat{T}$, which acts as a material configuration. The position, at some instant t, of the material points of the membrane associated to $\hat{T}$ is described by some injective, continuously differentiable function

$$\boldsymbol{\varphi}^t : \hat{T} \to \mathbb{R}^3 \tag{1}$$

In the finite element implementation this function is defined elementwise as a linear combination of basis functions on $\hat{T}$, i.e.,

$$\boldsymbol{\varphi}^t(\xi) = \sum_{m=1}^{M} \boldsymbol{X}_{(m)}(t) N_{(m)}(\xi) \tag{2}$$

where $\boldsymbol{X}_{(m)}(t)$ is the position, at time t, of the mth node of the element (we assume a Lagrangian finite element with M nodes for clarity). Notice that $\xi \in \mathbb{R}^2$.

The image of $\hat{T}$ by φ^t is denoted here by T^t. Because of the injectivity of $\boldsymbol{\varphi}^t$, it is possible to define the (also of class $\mathcal{C}^1$) inverse mapping

$$\boldsymbol{\psi}^t : T^t \to \widehat{T}, \quad \text{such that} \qquad \boldsymbol{\psi}^t(\boldsymbol{\varphi}^t(\xi)) = \xi \quad \forall \xi \in \widehat{T} \tag{3}$$

Without loss of generality, it is assumed that the relaxed configuration of the membrane corresponds to $t = 0$. The deformation of the membrane is thus characterized by the mapping

$$\zeta^t : T^0 \to T^t, \quad \text{defined by} \quad \zeta^t(\boldsymbol{x}) := \boldsymbol{\varphi}^t(\boldsymbol{\psi}^0(\boldsymbol{x})) \tag{4}$$

To compute the deformation gradient some additional work is needed, since the gradient of $\boldsymbol{\varphi}^t$ is, with cartesian coordinates for T^t, a 3×2-matrix and thus not invertible (if $\widehat{T}$ were an open set in $\mathbb{R}^3$, one would simply compute $\nabla\zeta^t(\boldsymbol{x}) = \nabla\boldsymbol{\varphi}^t(\boldsymbol{\psi}^0(\boldsymbol{x})) \left[\nabla\boldsymbol{\varphi}^0(\boldsymbol{\psi}^0(\boldsymbol{x}))\right]^{-1}$).

The tangential deformation gradient is a rank-2 tensor from the tangent plane at $\boldsymbol{x} = \boldsymbol{\varphi}^0(\xi)$ to the tangent plane at $\boldsymbol{y} = \zeta^t(\boldsymbol{x}) = \boldsymbol{\varphi}^t(\xi)$. Take a cartesian basis $(\check{\boldsymbol{e}}^{(1)}, \check{\boldsymbol{e}}^{(2)})$ at $\widehat{T}$, which is nothing but the canonical basis at the master element. Two linearly independent vectors $(\boldsymbol{G}^{(1)}, \boldsymbol{G}^{(2)})$ tangent to T^0 at $\boldsymbol{x}$ are defined as the infinitesimal images of the basis:

$$\boldsymbol{\varphi}^0(\xi + \epsilon_1\check{\boldsymbol{e}}^{(1)} + \epsilon_2\check{\boldsymbol{e}}^{(2)}) = \boldsymbol{\varphi}^0(\xi) + \epsilon_1\boldsymbol{G}^{(1)} + \epsilon_2\boldsymbol{G}^{(2)} + \mathcal{O}(\epsilon_1^2 + \epsilon_2^2) \tag{5}$$

and are calculated in cartesian components as

$$\left\{\boldsymbol{G}^{(i)}\right\}_j = \frac{\partial\varphi_j^0}{\partial\xi_i} = \sum_{m=1}^{M} X_{(m)j}(0)\frac{\partial N_{(m)}}{\partial\xi_i} \quad i = 1,2;\ j = 1,2,3 \tag{6}$$

the normal $\check{\boldsymbol{N}}$ to T^0 at $\boldsymbol{x}$ is given by

$$\check{\boldsymbol{N}} = \frac{\boldsymbol{G}^{(1)} \times \boldsymbol{G}^{(2)}}{\|\boldsymbol{G}^{(1)} \times \boldsymbol{G}^{(2)}\|} \tag{7}$$

thus defining an orthonormal basis of $\mathbb{R}^3$ such that its two first vectors are tangent to T^0 (and thus a basis of the tangent plane) as

$$\boldsymbol{V}^{(1)} = \frac{\boldsymbol{G}^{(1)}}{\|\boldsymbol{G}^{(1)}\|}, \quad \boldsymbol{V}^{(2)} = \check{\boldsymbol{N}} \times \boldsymbol{V}^{(1)}, \quad \boldsymbol{V}^{(3)} = \check{\boldsymbol{N}} \tag{8}$$

Analogous vectors can be defined at $\boldsymbol{y}$ by replacing $\boldsymbol{\varphi}^0$ with $\boldsymbol{\varphi}^t$ in the previous definitions. They will be denoted by lowercase letters: $\boldsymbol{g}^{(1)}$, $\boldsymbol{g}^{(2)}$, $\check{\boldsymbol{n}}$, $\boldsymbol{v}^{(1)}$, $\boldsymbol{v}^{(2)}$ and $\boldsymbol{v}^{(3)}$.

The tangential deformation gradient is thus given by the infinitesimal deformation (by ζ^t) of the vectors $\boldsymbol{V}^{(1)}$ and $\boldsymbol{V}^{(2)}$, which is given by

$$\zeta^t(\boldsymbol{x} + \epsilon_1\boldsymbol{V}^{(1)} + \epsilon_2\boldsymbol{V}^{(2)}) = \zeta^t(\boldsymbol{x}) + (\mathcal{F}_{11}\epsilon_1 + \mathcal{F}_{12}\epsilon_2)\boldsymbol{v}^{(1)} + (\mathcal{F}_{21}\epsilon_1 + \mathcal{F}_{22}\epsilon_2)\boldsymbol{v}^{(2)} + \mathcal{O}(\epsilon_1^2 + \epsilon_2^2) \tag{9}$$

where the matrix $\underline{\underline{\mathcal{F}}}$ is given by

$$\mathcal{F}_{11} = \frac{\|\boldsymbol{g}^{(1)}\|}{\|\boldsymbol{G}^{(1)}\|} \tag{10}$$

$$\mathcal{F}_{12} = \frac{\boldsymbol{g}^{(2)} \cdot \boldsymbol{v}^{(1)}}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}} - \frac{\|\boldsymbol{g}^{(1)}\|}{\|\boldsymbol{G}^{(1)}\|}\frac{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(1)}}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}} \tag{11}$$

$$\mathcal{F}_{21} = 0 \tag{12}$$

$$\mathcal{F}_{22} = \frac{\boldsymbol{g}^{(2)} \cdot \boldsymbol{v}^{(2)}}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}} \tag{13}$$

Remark 2.1. In fact, the left-hand side of (9) should read

$$\zeta^t\left(\boldsymbol{\Pi}_0(\boldsymbol{x} + \epsilon_1\boldsymbol{V}^{(1)} + \epsilon_2\boldsymbol{V}^{(2)})\right)$$

where $\boldsymbol{\Pi}_0 : \mathbb{R}^3 \to T^0$ is the closest-point projection onto T^0, because $\boldsymbol{x} + \epsilon_1\boldsymbol{V}^{(1)} + \epsilon_2\boldsymbol{V}^{(2)}$ does not belong to T^0 and thus ζ^t is not defined at it.

Eq. (9) defines the deformation-gradient tensor $\mathbb{F}^t$ which maps de tangent plane at $\boldsymbol{x} \in T^0$ onto the tangent plane at $\boldsymbol{y} \in T^t$ as the only linear operator satisfying, for all tangent vectors $\boldsymbol{t}$,

$$\zeta^t(\boldsymbol{\Pi}_0(\boldsymbol{x} + \epsilon\boldsymbol{t})) = \boldsymbol{y} + \epsilon\,\mathbb{F}^t\boldsymbol{t} + \mathcal{O}(\epsilon^2) \tag{14}$$

To prove that (14) indeed holds, one starts from the identities (true by construction)

$$\boldsymbol{g}^{(i)} = \mathbb{F}^t\boldsymbol{G}^{(i)} \quad i = 1,2 \tag{15}$$

so that, since $\mathcal{F}_{11}$ is, from (9), equal to

$$\mathcal{F}_{11} = \boldsymbol{v}^{(1)} \cdot \mathbb{F}^t\boldsymbol{V}^{(1)}$$

it results that

$$\mathcal{F}_{11} = \boldsymbol{v}^{(1)} \cdot \mathbb{F}^t\boldsymbol{V}^{(1)} = \frac{\boldsymbol{g}^{(1)}}{\|\boldsymbol{g}^{(1)}\|} \cdot \mathbb{F}^t\left(\frac{\boldsymbol{G}^{(1)}}{\|\boldsymbol{G}^{(1)}\|}\right) = \frac{\boldsymbol{g}^{(1)} \cdot \mathbb{F}^t\boldsymbol{G}^{(1)}}{\|\boldsymbol{g}^{(1)}\|\|\boldsymbol{G}^{(1)}\|} = \frac{\|\boldsymbol{g}^{(1)}\|}{\|\boldsymbol{G}^{(1)}\|}$$

From the identity $\boldsymbol{G}^{(2)} = \boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(1)}\boldsymbol{V}^{(1)} + \boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}\boldsymbol{V}^{(2)}$, applying $\mathbb{F}^t$ to both sides and rearranging, we obtain

$$\mathbb{F}^t\boldsymbol{V}^{(2)} = \frac{1}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}}\left(\boldsymbol{g}^{(2)} - \frac{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(1)}}{\|\boldsymbol{G}^{(1)}\|}\boldsymbol{g}^{(1)}\right)$$

and this yields

$$\mathcal{F}_{12} = \boldsymbol{v}^{(1)} \cdot \mathbb{F}^t\boldsymbol{V}^{(2)} = \frac{\boldsymbol{v}^{(1)} \cdot \boldsymbol{g}^{(2)}}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}} - \frac{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(1)}}{\boldsymbol{G}^{(2)} \cdot \boldsymbol{V}^{(2)}}\frac{\|\boldsymbol{g}^{(1)}\|}{\|\boldsymbol{G}^{(1)}\|}$$

The other two components of $\underline{\underline{\mathcal{F}}}$ are obtained similarly.

The right tangential Cauchy–Green tensor $\mathbb{C}^t = (\mathbb{F}^t)^T\mathbb{F}^t$, expressed in the basis $(\boldsymbol{V}^{(1)}, \boldsymbol{V}^{(2)})$, has components that are straightforward to calculate,

$$\underline{\underline{\mathcal{C}}}^t = \underline{\underline{\mathcal{F}}}^T\underline{\underline{\mathcal{F}}} = \begin{pmatrix} \mathcal{F}_{11}^2 & \mathcal{F}_{11}\mathcal{F}_{12} \\ \mathcal{F}_{11}\mathcal{F}_{12} & \mathcal{F}_{12}^2 + \mathcal{F}_{22}^2 \end{pmatrix} \tag{16}$$

and the Green–Saint Venant tensor $\mathbb{E}^t = (\mathbb{C}^t - \mathbb{I})/2$, in the same basis, is given by the matrix

$$\underline{\underline{\mathcal{E}}}^t = \frac{1}{2}\left(\underline{\underline{\mathcal{C}}}^t - \underline{\underline{\mathcal{I}}}\right) \tag{17}$$

with $\underline{\underline{\mathcal{I}}}$ the identity matrix. The energy density at $\boldsymbol{y} = \zeta^t(\boldsymbol{x})$ of an isotropic elastic material is a function of the invariants of $\underline{\underline{\mathcal{C}}}^t$ (such as its

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