Journal of Computational Physics 298 (2015) 565–584

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A semi-implicit finite element method for viscous lipid membranes

Diego S. Rodrigues, Roberto F. Ausas, Fernando Mut, Gustavo C. Buscaglia *

Instituto de Ciências Matemáticas e de Computação, Universidade de São Paulo, Av. do Trabalhador são-carlense, 400, 13566-590 São Carlos, SP, Brazil

ARTICLE INFO

Article history:
Received 27 June 2014
Accepted 7 June 2015
Available online 25 June 2015

Keywords:
Biological membranes
Lipid bilayer
Bending energy
Canham–Helfrich energy
Surface viscosity
Boussinesq–Scriven operator
Inextensibility
Tangential calculus
Surface finite elements

ABSTRACT

A finite element formulation to approximate the behavior of lipid membranes is proposed. The mathematical model incorporates tangential viscous stresses and bending elastic forces, together with the inextensibility constraint and the enclosed volume constraint. The membrane is discretized by a surface mesh made up of planar triangles, over which a mixed formulation (velocity–curvature) is built based on the viscous bilinear form (Boussinesq–Scriven operator) and the Laplace–Beltrami identity relating position and curvature. A semi-implicit approach is then used to discretize in time, with piecewise linear interpolants for all variables. Two stabilization terms are needed: The first one stabilizes the inextensibility constraint by a pressure–gradient–projection scheme (Codina and Blasco (1997) [33]), the second couples curvature and velocity to improve temporal stability, as proposed by Bänsch (2001) [36]. The volume constraint is handled by a Lagrange multiplier (which turns out to be the internal pressure), and an analogous strategy is used to filter out rigid-body motions. The nodal positions are updated in a Lagrangian manner according to the velocity solution at each time step. An automatic remeshing strategy maintains suitable refinement and mesh quality throughout the simulation.

Numerical experiments show the convergent and robust behavior of the proposed method. Stability limits are obtained from numerous relaxation tests, and convergence with mesh refinement is confirmed both in the relaxation transient and in the final equilibrium shape. Virtual tweezing experiments are also reported, computing the dependence of the deformed membrane shape with the tweezing velocity (a purely dynamical effect). For sufficiently high velocities, a tether develops which shows good agreement, both in its final radius and in its transient behavior, with available analytical solutions. Finally, simulation results of a membrane subject to the simultaneous action of six tweezers illustrate the robustness of the method.

1. Introduction

Phospholipid membranes are two-molecule-thick surface arrays of phospholipids [1] that constitute the fundamental building material of the Living Cell membrane, of many intra-cellular units, and of synthetic vesicles such as liposomes. The static properties of this two-dimensional material are governed by geometry. In fact remarkable agreement with biophysical

* Corresponding author.
E-mail addresses: diegosarodrigues@gmail.com (D.S. Rodrigues), rfausas@icmc.usp.br (R.F. Ausas), fermut@gmail.com (F. Mut), gustavo.buscaglia@icmc.usp.br (G.C. Buscaglia).

http://dx.doi.org/10.1016/j.jcp.2015.06.010
0021-9991/

observations has been obtained with models in which the energy density (per unit area) is a function of the local curvature alone [2,3]. Such an energy density is typical of thin *elastic solids* in bending.

Numerical methods for computing equilibrium shapes of these membranes by gradient flow (which in this context is called *Willmore flow*) first appeared about ten years ago, with the works of Dziuk [4], Rusu [5], Feng and Klug [6] and Barrett et al. [7], among others. These methods evolve the geometry by gradient descent towards an equilibrium of the applied forces (if any) with the elastic forces. Bonito et al. [8,9] considered the effect of the bulk fluid, while Elliot and Stinner modeled two-phase effects [10], both of them without modeling the membrane's tangential rheology.

The actual dynamics of phospholipid membranes does not obey gradient flow. Their evolution results from the interplay between the applied forces, the hydrodynamic forces coming from the adjacent inner and outer liquids, and the forces that develop on the membrane itself, which include an elastic contribution (as in gradient flow) and also a surface viscous contribution arising from the lipid-to-lipid sliding. In this article we focus just on the membrane forces, restricting the effect of the adjacent liquids to just a volume constraint. The combination of the methods proposed below with more realistic treatments of the inner and outer liquids is straightforward (though the added computational cost is obviously significant).

We assume that the surface viscous forces that develop on the membrane and determine its dynamics correspond to an area-preserving *Newtonian surface fluid* [11–13]. Our goal is thus to present a finite element method for the *viscous flow* of phospholipid bilayers; i.e., for the dynamical simulation of phospholipid bilayers, considering an elastic model for bending deformations and a (viscous) Newtonian area-preserving fluid model for the dissipative tangential motions.

For this purpose, we adopt the same treatment of elastic forces used for gradient flows [4,8], combined with a novel treatment of surface viscous forces. The mathematical formulation of surface viscous behavior was first derived by Scriven [14]. Schemes for its numerical approximation have been proposed by Arroyo and coworkers [13,15,16] in the axisymmetric case, and by Tasso and Buscaglia [17] in the general 3D case. The formulation of this latter article relies heavily on the numerical differentiation of the energy of the membrane (including an "evanescent elasticity" term which accounts for tangential viscosity) to compute forces and stresses, and on yet another numerical differentiation to compute the approximate tangent matrix. In this work another approach is followed, developing a semi-implicit scheme issued in a classical way from the continuous variational formulation, without adjustable numerical differentiation parameters and involving the solution of just one linear system per time step.

After introducing the mathematical formulation in Section 2 and the proposed discretization scheme in Section 3, we assess the proposed method through numerical examples in Section 4. Special attention is given to experiments that involve membrane tweezing and tether formation. The latter is a salient phenomenon that takes place in phospholipid bilayers, by which if a small part of a vesicle is pulled away by some localized force (using an optical trap, for example [18–20]) it carries with it a narrow bilayer tube (tether) that can be much longer than the vesicle itself and nanometric in diameter [21]. The proposed method is shown to be sufficiently robust to allow for accurate simulations of tether formation and extension, which are important to shed light on fundamental mechanisms of cell mechanics [22–24]. Section 5 is then devoted to summarize the conclusions of the study.

2. Mathematical formulation

2.1. Virtual power at the interface

We consider the motion of a closed surface $\Gamma \subset \mathbb{R}^3$ under the action of surface elastic forces and external forces coming from the adjacent liquid. The virtual work principle for such a system reads

$$\int_\Gamma \boldsymbol{\sigma} : D_\Gamma \mathbf{v} = -d\mathcal{E}(\mathbf{v}) + \int_\Gamma \mathbf{f}\cdot\mathbf{v} \qquad \forall \mathbf{v} \in \mathbf{V}\,, \tag{1}$$

where $\boldsymbol{\sigma}$ is the tensor of tangential stresses, $\mathcal{E}(\Gamma)$ is the elastic energy from which elastic forces are derived, $\mathbf{f}$ is the net interaction force with the surroundings, $\mathbf{V}$ the space of admissible virtual velocities and $D_\Gamma\mathbf{v}$ the surface virtual strain rate.

In (1), by $d\mathcal{E}(\mathbf{v})$ we denote the derivative (or first variation) of $\mathcal{E}(\Gamma)$ along the virtual velocity field $\mathbf{v}$. In turn, $D_\Gamma\mathbf{v}$ represents the surface differential operator

$$D_\Gamma \mathbf{v} = \frac{1}{2}\,\mathbb{P}\,(\nabla_\Gamma \mathbf{v} + \nabla_\Gamma \mathbf{v}^T)\,\mathbb{P}\,, \tag{2}$$

which is the surface analog of the usual three-dimensional symmetric gradient $D\mathbf{v} = (\nabla\mathbf{v} + \nabla\mathbf{v}^T)/2$.

Some elements of differential geometry are needed at this point. We follow the presentation of Buscaglia and Ausas [25], the reader is also referred to Biria et al. [26] for a more comprehensive review.

The tensor $\mathbb{P}$ above is the tangent projector onto Γ given by

$$\mathbb{P} = \mathbb{I} - \breve{\mathbf{n}} \otimes \breve{\mathbf{n}}, \tag{3}$$

$\breve{\mathbf{n}}$ being the outward normal to Γ, and the symbol ∇_Γ refers to the surface gradient, given by

$$\nabla_\Gamma f = \mathbb{P}\,\nabla \widehat{f}\,, \tag{4}$$