Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2015-0029

Vol. **21**, No. 1, pp. 40-64
January 2017

Fast Simulation of Lipid Vesicle Deformation Using Spherical Harmonic Approximation

Michael Mikucki[1] and Yongcheng Zhou[2,*]

[1] *Department of Applied Mathematics & Statistics, Colorado School of Mines, Golden, Colorado, 80401, USA.*
[2] *Department of Mathematics, Colorado State University, Fort Collins, Colorado, 80523, USA.*

Received 24 December 2015; Accepted (in revised version) 26 May 2016

Abstract. Lipid vesicles appear ubiquitously in biological systems. Understanding how the mechanical and intermolecular interactions deform vesicle membranes is a fundamental question in biophysics. In this article we develop a fast algorithm to compute the surface configurations of lipid vesicles by introducing surface harmonic functions to approximate the membrane surface. This parameterization allows an analytical computation of the membrane curvature energy and its gradient for the efficient minimization of the curvature energy using a nonlinear conjugate gradient method. Our approach drastically reduces the degrees of freedom for approximating the membrane surfaces compared to the previously developed finite element and finite difference methods. Vesicle deformations with a reduced volume larger than 0.65 can be well approximated by using as small as 49 surface harmonic functions. The method thus has a great potential to reduce the computational expense of tracking multiple vesicles which deform for their interaction with external fields.

AMS subject classifications: 35Q92, 92C40, 65M70

Key words: Lipid bilayer, curvature energy, surface harmonics, fast algorithm.

1 Introduction

This paper describes a fast numerical algorithm for computing the configuration of lipid bilayer vesicles. Lipid bilayers are crucial components to living systems. Being amphiphilic, lipid molecules have charged or polar hydrophilic head groups and hydrophobic tails. This allows lipids in aqueous solution to aggregate into structures that entropically favor the alignment of hydrophobic tails and the exposure of hydrophilic head

*Corresponding author. *Email addresses:* mikucki@mines.edu (M. Mikucki), yzhou@math.colostate.edu (Y. Zhou)

groups to water. A lipid bilayer is formed from the self-assembly of hydrophobic tails of the two complementary layers. The bilayer will then close so the hydrophobic core will not be exposed at the free edges, forming membranes of cells and sub-cellular organelles. These membranes are semi-permeable boundaries separating the enclosure from the surrounding environment. At the microscale, lipid bilayer membranes regulate the transportation of ions, proteins, and other molecules between separated domains, and provide a flexible platform on which molecules can aggregate to carry out vital chemical or physical reactions. At the mesoscale, for example, membranes of the red blood cells (RBCs) suspended in blood flow change their shape in response to the local flow conditions, and this change will in turn affect the RBC's ability of oxygen transport and the hydrodynamic properties of the blood flow [1,10]. Deformation of the bilayer membranes are driven by various types of force, which may dominate at different length scales. At the microscale, driven forces are mainly the results of protein-membrane or membrane-membrane interactions, such as protein binding or insertion, lipid insertion or translation, and ubiquitous electrostatic interactions, to name a few [13]. At the mesoscale, hydrodynamic forces usually dominate [5, 18, 36]. Determination of the membrane geometry in response to protein-membrane, membrane-membrane, or fluid-membrane interactions is necessary for elucidating the structure-function relation of these interacted biological systems.

The variation of lipid bilayer configurations can be characterized by its deformation energy. This energy is the handle of almost all computational methods. Classical strain energy can be defined for lipid bilayers so their deformation can be described as elastic plates [43]. A crucial difference between the plates and bilayer membranes is missing in such models: a flat membrane can be subject to some shear deformation with zero energy cost provided the deformation is so slow that the viscous effect of lipids is negligible [26]. As a result, the deformation energy of a lipid bilayer is mostly attributed to the bending energy of the monolayers. The classical energy forms proposed by Canham [3], Helfrich [17], and Evans [11], are of this type, in which the deformation energy is defined be a quadratic function of the principle curvature of the surface. Other components of the energy, such as those corresponding to the area expansion and contraction of the monolayers, and the osmotic pressure, are of several orders of magnitude larger than the bending energy, and usually serve in computational models as area and enclosed volume constraints of the bilayer membrane, respectively. With this simplification, often referred to as the spontaneous curvature model, the deformation energy of the bilayer membrane is given by the bending curvature equation with two constraints. The equilibrium configuration of lipid bilayer vesicles can be obtained by minimizing this energy. For sufficiently simplified membrane systems such as isolated vesicles with symmetric lipid composition, analytical analysis of these energies can give an excellent classification of the phases of the vesicle configurations, particularly the axisymmetric configurations, and can accurately locate the conditions under which the phase transition occurs [28, 29, 42]. Giving the complexity the realistic interacted biological system with which lipid bilayer is interacted, analytical approaches may fail in quantifying these interactions and thus