Journal of Computational Physics 354 (2018) 67–85

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Unconditionally energy stable numerical schemes for phase-field vesicle membrane model

F. Guillén-González [a], G. Tierra [b,*]

[a] Departamento de Ecuaciones Diferenciales y Análisis Numérico & IMUS, Universidad de Sevilla, Aptdo. 1160, 41080 Seville, Spain
[b] Department of Mathematics, Temple University, Philadelphia PA 19122, USA

ARTICLE INFO

Article history:
Received 19 May 2017
Received in revised form 27 October 2017
Accepted 31 October 2017
Available online 3 November 2017

Keywords:
Diffuse interface phase-field
Cahn–Hilliard
Bending energy
Vesicle membrane
Energy stability
Multiphase flow
Splitting schemes

ABSTRACT

Numerical schemes to simulate the deformation of vesicles membranes via minimizing the bending energy have been widely studied in recent times due to its connection with many biological motivated problems. In this work we propose a new unconditionally energy stable numerical scheme for a vesicle membrane model that satisfies exactly the conservation of volume constraint and penalizes the surface area constraint. Moreover, we extend these ideas to present an unconditionally energy stable splitting scheme decoupling the interaction of the vesicle with a surrounding fluid. Finally, the well behavior of the proposed schemes are illustrated through several computational experiments.

1. Introduction

Biological vesicle membranes are closed structures made of two opposed lipid monolayers with anchored proteins that separates two aqueous compartments. The study of formation and dynamics of vesicle membranes has been an active source of experimental and theoretical investigations in biology, biophysics and bioengineering for the past several decades (see [5,4] and the references therein). The morphological changes of vesicles presents interesting challenges to carry out efficient and accurate numerical simulations, effective mathematical modeling and rigorous analysis due to the variety of equilibrium shapes assumed by vesicles in biological experiments, that correspond with minimizers of different surface energies, such as the bending elastic energy [1]. However, in studying structural changes and deformation of vesicles, one must additionally understand the coupling of these configurations with external fields [2,24].

In recent times, many works have focused on designing and studying numerical approximations of this type of models. In [10,11], the authors present several numerical simulations where the physical constraints are imposed by using a penalized formulation and Lagrange multipliers respectively. Numerical analysis and error estimates for a saddle point formulation with the constraints approximated via Lagrange multipliers is presented in [14]. For the case of considering a penalized formulation of the constraints, existence and uniqueness results of the global weak solutions are established in [8]. Moreover, in [7] the authors present the convergence to equilibrium of global weak solutions for a Cahn–Hilliard–Navier–Stokes vesicle model with penalized surface area constraint. In [12], the authors present a study of numerical approximations of the vesicle membrane deformations considering both approximations of the constraints (penalization approach and Lagrange

* Corresponding author.
E-mail addresses: guillen@us.es (F. Guillén-González), gtierra@temple.edu (G. Tierra).

https://doi.org/10.1016/j.jcp.2017.10.060
0021-9991/

multipliers), where the convergence of the numerical schemes towards the continuous problems and some numerical experiments are presented. A three-dimensional adaptive finite element method is developed in [13] where the effectiveness of the adaptive method is demonstrated through numerical examples. For a study of a phase field model developed for vesicle adhesion involving complex substrate we refer the reader to [31]. In [6] the authors propose an unconditionally energy stable scheme for the vesicle membrane model but they only impose the constraint of conservation of volume, skipping the difficulties related with imposing the surface area constraint. In [29] the authors study the problem where the constraints of conservation of mass and volume are penalized, proposing a linear energy stable scheme with respect to a modified energy, although it is not clear that this approach will imply energy stability with respect to the original energy.

The paper is organized as follows: In Section 2 we present the model that we are considering and a reformulation of the problem that allows to easily derive the energy law of the system. Section 3 is devoted to design a new numerical scheme and show its unconditionally energy stability, its well-posedness and its convergence. In Section 4 we present several numerical experiments in order to show the validity of our approach and to show the dynamics of the system. Finally, we state the conclusions of our work in Section 5.

2. The model

We consider the model derived in [9] to approximate the deformation of membrane-bound vesicles by means of an incompressible flow and phase field coupling. The idea is to introduce a phase function $\phi(x)$, defined on the spatial domain $\Omega \subset \mathbb{R}^3$, which is used to label the inside and the outside of the vesicle.

We consider a phase field variable ϕ which is used to localize the membrane, taking one value inside the vesicle (for instance $\phi = 1$) and another value outside the vesicle (for instance $\phi = -1$). The corresponding interface motion is derived through the energetic variational approach with respect to a *bending energy* $E_b(\phi)$ associated to the phase field function with $\varepsilon > 0$ related with the interfacial width. In particular, the bending energy is defined as

$$E_b(\phi) := \frac{\varepsilon}{2}\int_\Omega \left(\Delta\phi - \frac{1}{\varepsilon^2}G(\phi)\right)^2 d\boldsymbol{x} = \frac{\varepsilon}{2}\int_\Omega \omega^2 d\boldsymbol{x}, \tag{2.1}$$

where

$$\omega := -\Delta\phi + \frac{1}{\varepsilon^2}G(\phi), \qquad G(\phi) := F'(\phi) - \varepsilon k(\boldsymbol{x})H'(\phi) \tag{2.2}$$

with

$$F(\phi) := \frac{1}{4}(\phi^2-1)^2, \quad H(\phi) := \frac{1}{3}\phi^3 - \phi,$$

and $k(\boldsymbol{x})$ is a given function representing the spontaneous curvature. The vesicle volume and surface area are defined as

$$A(\phi) := \int_\Omega \phi\, d\boldsymbol{x} \quad \text{and} \quad B(\phi) := \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi)\right) d\boldsymbol{x},$$

respectively. Due to the fact that the volume $A(\phi)$ and the surface area $B(\phi)$ of the vesicles have to remain constant in time, it is necessary to take into account how to enforce these two constraints while the numerical schemes are developed. The volume conservation will be imposed exactly by considering a H^{-1}-gradient flow (Cahn–Hilliard-type model) while the conservation of the surface area will be approximated via penalization.

2.1. Cahn–Hilliard type model for the behavior of a vesicle membrane

The model to study deformation of vesicle membranes can be derived from the bending energy (2.1) as the Cahn–Hilliard equation in $(0,+\infty)\times\Omega$:

$$\phi_t - \nabla\cdot\left(\gamma\,\nabla\left(\frac{\delta E_b}{\delta\phi}\right)\right) = 0, \tag{2.3}$$

where $\gamma > 0$ is a mobility parameter and

$$\frac{\delta E_b}{\delta\phi} = \varepsilon\Big(-\Delta\omega + \frac{1}{\varepsilon^2}G'(\phi)\omega\Big) = -\varepsilon\Delta\omega + \frac{1}{\varepsilon}G'(\phi)\omega.$$

In particular, this system supplemented with adequate boundary conditions satisfies a dissipative energy law (testing (2.3) by $\delta E_b/\delta\phi$):

$$\frac{d}{dt}E_b(\phi(t)) + \gamma\left\|\nabla\left(\frac{\delta E_b}{\delta\phi}\right)\right\|^2_{L^2(\Omega)} = 0, \quad \forall t > 0.$$