Journal of Computational Physics 302 (2015) 509–523

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Decoupled energy stable schemes for phase-field vesicle membrane model

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ARTICLE INFO

Article history:
Received 9 March 2015
Received in revised form 12 September 2015
Accepted 14 September 2015
Available online 25 September 2015

Keywords:
Phase-field
Multiphase flows
Vesicle membrane
Navier–Stokes
Allen–Cahn
Stability

ABSTRACT

We consider the numerical approximations of the classical phase-field vesicle membrane models proposed a decade ago in Du et al. (2004) [6]. We first reformulate the model derived from an energetic variational formulation into a form which is suitable for numerical approximation, and establish the energy dissipation law. Then, we develop a stabilized, decoupled, time discretization scheme for the coupled nonlinear system. The scheme is unconditionally energy stable and leads to linear and decoupled elliptic equations to be solved at each time step. Stability analysis and ample numerical simulations are presented thereafter.

1. Introduction

In cell biology, a vesicle is a small organelle within a cell, consisting of fluid enclosed by a lipid bilayer membrane. There have been many experimental and analytic studies on the configurations and deformations of elastic vesicle biomembranes [2,6,12–14,17]. In the last decade, using the energetic, variational diffuse interface approach, Du et al. proposed a phase-field model to simulate the deformations of simple vesicles coupled with incompressible flow fields [6–8,10], in which, the Helfrich bending elastic energy of the surface is replaced by a phase field functional. The evolution equations are then resulted from the variations of the action functional of the free energy.

The diffuse-interface/phase-field models, whose origin can be traced back to [9,33], have been proved efficient with much success. A particular advantage of the phase-field approach is that they can often be derived from an energy-based variational formalism, leading to well-posed nonlinear coupled systems that satisfy thermodynamics-consistent energy dissipation laws. Thus it is especially desirable to design numerical schemes that preserve the energy dissipation law at the discrete level. Due to the rapid changes near the interface, the non-compliance of energy dissipation laws of the numerical scheme may lead to spurious numerical solutions if the grid and time step sizes are not carefully controlled [11,21]. Another main advantage of energy stable schemes is that they can be easily combined with an adaptive time stepping strategy [22–24,26–28,35].

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http://dx.doi.org/10.1016/j.jcp.2015.09.025
0021-9991/

To construct the numerical schemes for the typical phase-field models coupled with the hydrodynamics, in particular, the Allen–Cahn or Cahn–Hilliard equations, the main difficulties include (i) the coupling between the velocity and phase function through the convection term in the phase equation and nonlinear stress in the momentum equation; (ii) the coupling of the velocity and pressure through the incompressibility constraint; (iii) the stiffness of the phase equation associated with the interfacial width. For the phase-field vesicle membrane model [6–8,10], things are about to get even worse due to some extra nonlinear terms with second order derivatives. To the best of the authors' knowledge, there does not exist any easy-to-implement and energy stable scheme for this model so far.

Thus, for the phase-field membrane vesicle model, the main purpose of this paper is to construct a time discretization scheme which (a) satisfies a discrete energy law; and (b) leads to decoupled elliptic equations to solve at each time step. This is by no means an easy task due to many highly nonlinear terms and the couplings among the velocity, pressure and phase function.

The rest of the paper is organized as follows. In Section 2, we introduce the phase-field vesicle membrane model and derive the energy dissipation law. In Section 3, we reformulate the PDE to an equivalent form, construct a decoupled, energy stable numerical scheme, and give the stability analysis. In Section 4, we present the spatial discretization using the finite element method. In Section 5, we present some numerical results to illustrate the accuracy and efficiency of the proposed scheme and summarize our contributions. Some concluding remarks are given in Section 6.

2. Models

The equilibrium shape of a vesicle membrane is determined by minimizing the elastic bending energy [3,4],

$$E = \int_\Gamma (a_1 + a_2(H - c_0)^2 + a_3 K)ds, \tag{2.1}$$

where $H = \dfrac{k_1 + k_2}{2}$ represents mean curvature of the membrane surface; $K = k_1 k_2$ is Gaussian curvature; k_1, k_2 are two principle curvatures; a_1 is the surface tension; a_2, a_3 are bending rigidities; c_0 represents spontaneous curvature; Γ is a smooth compact surface in the domain $\Omega \in \mathbf{R}^3$.

If we consider the model to be isotropic, i.e., the spontaneous curvature $c_0 = 0$ and neglect the constants a_1 and a_3 due to the Gauss–Bonnet formula, then the elastic bending energy can be written by,

$$E = \int_\Gamma \frac{K}{2} H^2 ds. \tag{2.2}$$

In the framework of phase-field method, a variable $\phi(x) = \tanh\left(\dfrac{d(x)}{\sqrt{2}\epsilon}\right)$ is defined for all $x \in \Omega$, where $d(x)$ is the signed distance between a point x and Γ, positive inside and negative outside; ϵ is a transition parameter that is taken to be very small. Thus $H = -\dfrac{1}{2} tr(\nabla^2 d(x))$ on the surface and one can obtain the bending energy as follows [8],

$$E_b = \int_\Omega \frac{\epsilon}{2} |\Delta\phi - f(\phi)|^2 dx, \tag{2.3}$$

where $F(\phi) = \dfrac{(\phi^2 - 1)^2}{4\epsilon^2}$ is the Ginzburg–Landau double well potential, $f(\phi) = F'(\phi)$ and ϵ is penalty parameter.

If one considers the constraints of the volume and the surface area, then the energy functional E_b includes two extra terms as follows [6,10],

$$E_b = \int_\Omega \frac{\epsilon}{2} |\Delta\phi - f(\phi)|^2 dx + \frac{1}{2} M_1 (A(\phi) - \alpha)^2 + \frac{1}{2} M_2 (B(\phi) - \beta)^2, \tag{2.4}$$

where

$$A(\phi) = \int_\Omega \phi(x) dx, \quad B(\phi) = \int_\Omega \epsilon \left(\frac{1}{2} |\nabla\phi|^2 + F(\phi)\right) dx, \tag{2.5}$$

where $A(\phi)$ denotes the volume fractions, $B(\phi)$ is approaching a value of $2\sqrt{2}/3$ times of superficial area of the phase, M_1 and M_2 are the positive penalty parameters, α and β denote the constants of the volume and surface area, respectively.

Assuming the system is a vesicle bounded by incompressible fluid flows, the total energy E_{tot} of the hydrodynamic system is a sum of the kinetic energy E_k and the bending energy E_b, i.e.,

$$E_{tot} = E_k + \lambda E_b = \int_\Omega \frac{1}{2} \rho |\mathbf{u}|^2 dx + \lambda E_b, \tag{2.6}$$

where ρ is the density, $\mathbf{u}$ is the velocity, λ is the surface tension parameter.