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VESICLE SHAPE DEFORMATION USING A DISCONTINUOUS GALERKIN METHOD

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Abstract. This work concerns the development of a finite-element algorithm to discretize the phase-field model for the shape deformation of a vesicle based on the idea of discontinuous Galerkin method. The phase-field model originated from minimization of Canham-Helfrich elastic bending energy involves fourth-order gradients and thus C^1-basis functions are required for the standard conforming Galerkin formulation. We introduce a relatively inexpensive, nonconforming method based on C^0-basis functions. We present the variational form of the method including additional terms to weakly enforce continuity of the derivatives across interelement boundaries and its stabilization is achieved via Nitsche's method. Numerical tests for the equilibrium shape of a single component vesicle are performed to demonstrate the performance of the proposed variational formulation.

1 INTRODUCTION

Vesicles are simple forms of closed biomembranes. They are formed by bilayers of lipid molecules with a few nanometers thick ranging between 50 nm to tens of micrometers in diameter [1]. They are essential for many biological functions such as regulating protein activity and replication of viruses [2]. The objective of this study is to model the shape deformation of a vesicle using a C^0-discontinuous Galerkin formulation based on a phase-field bending elasticity model.

We employ the phase-field model originated from minimization of Canham-Helfrich elastic energy [3, 4] for modeling the shape deformation of vesicles. One of the main attractions of the phase-field model is its capability of easily incorporating the complex topological and geometrical changes without the explicit tracking of the interfaces. The phase-field model involves fourth-order partial derivatives. As a result, a standard Galerkin approximation requires C^1-continuous basis functions such that the phase-field variable and its first derivatives are continuous. Examples include Hermite elements and B-splines. Using Hermite elements on unstructured meshes presents difficulties and certain partitions are not permissible with their isoparametric versions [5]. The use of B-splines with arbitrarily shaped domains often involves either a mapping (as with isogeometrics) or a 'fictitious-domain' type of approaches [6]. More importantly, B-splines are non-interpolatory and, thus, imposing even simple Dirichlet boundary conditions can be problematic. Mixed finite-element methods present a relatively expensive alternative, requiring separate approximations for primary and secondary fields [7]. In this study, we present a finite-element formulation based on C^0-elements that can avoid these drawbacks.

The challenge of modeling the vesicle shape deformation using the phase-field model is high computational cost. This is because the phase-field is defined on the whole physical domain and it changes rapidly only near the transition layer around the vesicle membrane surface. Therefore, the use of adaptive meshing is more ideal than using uniform meshes on the whole domain. Bearing in mind this, developing efficient finite-element methods is important to model the shape deformation of the vesicle. Several methods have been developed, for example, an adaptive mixed method [8] and B-spline based finite-element method [9]. We expect that application of adaptivity to our proposed C^0-elements based finite-element formulation can be easily achieved.

The main goal of the paper is to present a variational formulation using C^0-elements to discretize the nonlinear fourth-order phase-field model for the shape deformation of vesicles. We employ Nitsche's [10] method to weakly impose continuity of the derivatives across element interfaces. An additional penalty like term is incorporated to achieve stabilization. Nitsche's method was first employed to develop a nonconforming finite-element formulation for a fourth-order elliptic problem by Baker [12]. Our approach is relevant to a consistent C^0-interior penalty method that was presented for beam and plate theories [11] and a second-gradient theory [13, 14, 16, 15]. Recently, Nitsche's method has been also successfully applied for weakly imposing Dirichlet boundary conditions in standard finite-element methods for second- and fourth-order partial differential equations [17, 18] and B-splines [19, 20].

The remainder of the paper is organized as follows. In Section 2, we briefly present the phased-field model for the equilibrium shape of vesicles. In Section 3, we introduce a variational formulation based on Nitsche's method for the phase-field model [31]). In Section 4, the capability of the proposed variational formulation is tested with a bi-concave shape example. Finally, in Section 5, we provide conclusions and a summary of directions for future work.

2 GOVERNING EQUATION

In the present work, we use the phase-field model of the Canham-Helfrich curvature energy [3, 4] for easy tracking of the shape deformation of the membrane surface. In doing so, we first introduce a phase-field function $\phi(x)$ on the computational domain Ω as in Du and his colleagues [8, 21, 22]. We visualize that the level set $\{x : \phi(x) = 0\}$ gives the membrane surface S, while $\{x : \phi(x) < 0\}$ represents the inside of the membrane and $\{x : \phi(x) > 0\}$ the outside. The equilibrium shape of the vesicle membrane is determined by minimizing its shape energy, usually taken to be its bending energy.

To derive the phase-field model, we introduce the phase-field bending energy [21, 22] given by

$$E(\phi) = \int_{\Omega} \frac{1}{2}\kappa\epsilon \left(\Delta\phi - \frac{1}{\epsilon^2}(\phi^2 - 1)(\phi + C\epsilon) \right)^2 \mathrm{d}v \tag{1}$$

where ϵ is the transition parameter related to the interface thickness and C is the parameter representing the effect of the spontaneous curvature. Then, the phase-field model for the equilibrium shape of a vesicle can be given by minimizing the energy (1) subject to the prescribed surface area and bulk volume. We employ the work of Du and colleagues [8, 21, 22] for the prescribed volume and area constraints. In doing so, we define

$$V(\phi) = \frac{1}{2}\left(\int_{\Omega} \phi(x)\, \mathrm{d}v \right) \tag{2}$$

for the prescribed volume constraint and

$$A(\phi) = \frac{3}{2\sqrt{2}} \int_{\Omega} \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 \right] \mathrm{d}v \tag{3}$$

for the prescribed surface area. We also consider the following initial phase-field function,

$$\phi(x) = \tanh\left(\frac{d(x, S)}{\sqrt{2}\epsilon} \right), \tag{4}$$

that was commonly used by Du and his colleagues [8, 21, 22]. Here, $d(x, S)$ is the signed distance function from a point $x \in \Omega$ to the membrane surface S.

To deal with surface area and volume constraints, we employ the following penalty formulation [8]

$$E_{\mathrm{P}}(\phi) = E(\phi) + \frac{\alpha_v}{2}(V(\phi) - V_0)^2 + \frac{\alpha_a}{2}(A(\phi) - A_0)^2 \tag{5}$$

where V_0 and A_0 represent the prescribed volume and the prescribed surface area and α_v and α_a are the penalty parameters. The problem to find equilibrium configurations of a vesicle membrane can be formulated as finding the phase-field function $\phi(x)$ on the whole domain Ω that minimizes the energy functional (5).

To find a minimizer of the energy (5), we employ a gradient flow approach that has been successfully used for solving the phase-field model of single-component vesicles [8, 21, 22]. Then, the variational problem can be solved via the gradient flow

$$\frac{\partial \phi}{\partial t} = -\frac{\delta E_{\mathrm{P}}(\phi)}{\delta \phi} \tag{6}$$

where $\delta/\delta\phi$ denotes the first variation of the functional (5). By taking the first variation of (5) and substituting it into the right-hand side of (6), (6) can be rewritten as

$$\begin{aligned}\frac{\partial \phi}{\partial t} = \Delta Q - \frac{1}{\epsilon^2} Q(3\phi^2 + 2C\epsilon\phi - 1) + \alpha_v(V(\phi) - V_0) + \\ \alpha_a(A(\phi) - A_0)\left[-\frac{3}{2\sqrt{2}}\epsilon\left(\Delta\phi - \frac{1}{\epsilon^2}(\phi^2 - 1)\phi\right)\right]\end{aligned} \tag{7}$$

where $Q = \epsilon\Delta\phi - \frac{1}{\epsilon}(\phi^2 - 1)(\phi + C\epsilon)$. To find the equilibrium shape of the vesicle, we use the time-dependent flow equation (7) with the initial phase-field function (4). Notice that it is the nonlinear and fourth order time-dependent partial differential equation and thus requires the nonlinear solver and an appropriate time-stepping algorithm.

To construct the weak form of (7), we introduce the space of an admissible solution field as $\mathcal{V} \subset H^2(\Omega)$, where $H^2(\Omega)$ denotes the classical Sobolev space of order 2. For convenience, we define the space of a test field as $\mathcal{W} \subset H^2(\Omega)$ with

$$\mathcal{W} = \{w \in H^2(\Omega) \mid w = \nabla w \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega\}. \tag{8}$$

By multiplying a test function $w \in \mathcal{W}$, taking integration over Ω, and applying integration by parts, the weak form to (7) can be stated as: Find $\phi \in \mathcal{V}$ such that, for all $w \in \mathcal{W}$,

$$\begin{aligned}\int_\Omega w\frac{\partial \phi}{\partial t}\,\mathrm{d}v = \epsilon\int_\Omega \Delta w\Delta\phi\,\mathrm{d}v + \frac{2}{\epsilon}\int_\Omega(\nabla w\cdot\nabla\phi)(3\phi^2 + 2C\epsilon\phi - 1)\,\mathrm{d}v \\ + \frac{1}{\epsilon}\int_\Omega w(6\phi + 2C\epsilon)(\nabla\phi\cdot\nabla\phi)\,\mathrm{d}v \\ + \frac{1}{\epsilon^3}\int_\Omega w(3\phi^2 + 2C\epsilon\phi - 1)(\phi^2 - 1)(\phi + C\epsilon)\,\mathrm{d}v \\ + \alpha_a\int_\Omega w(A(\phi) - A_0)\left[-\frac{3}{2\sqrt{2}}\epsilon\left(\Delta\phi - \frac{1}{\epsilon^2}(\phi^2 - 1)\phi\right)\right]\,\mathrm{d}v \\ + \alpha_v\int_\Omega w(V(\phi) - V_0)\,\mathrm{d}v.\end{aligned} \tag{9}$$

Notice that (9) is H^2-conforming and thus it is valid for C^1-continuous basis functions such as Hermite elements and B-splines.

3 C^0-DISCONTINUOUS GALERKIN FORMULATION

We present the non-conforming formulation based on the idea of Engel et al. [11]. This formulation uses C^0-continuous basis functions so that their first derivatives are discontinuous. Continuity of these first derivatives on element boundaries is weakly imposed based on Nitsche's method [10].

To construct the bases, we consider a regular finite-element partition $\Omega^h = \cup_{i=1}^{N} \Omega_i$, with $\Omega^h \approx \Omega$ and N the total number of elements in the mesh. We choose an approximation function $\phi_h \in \mathcal{V}^h$ which is continuous on the entire domain but discontinuous in its first and higher derivatives across element boundaries. Notice that $\mathcal{V}^h$ is a non-conforming approximation of $\mathcal{V}$, i.e., $\mathcal{V}^h \not\subset \mathcal{V}$. The approximation $\phi_h(\mathbf{x})$ to the phase-field function $\phi(\mathbf{x})$ is given by

$$\phi_h(\mathbf{x}) = \sum_I N_I(\boldsymbol{\xi}(\mathbf{x}))\phi_I \tag{10}$$

where ϕ_I is the nodal value at node I and $\boldsymbol{\xi}(\mathbf{x})$ is the position in a reference element. Here, N_I is a basis function that belongs to the set of Lagrangian iso-parametric functions

$$\{N_I\} = \{N_I \in C^0(\Omega^h) : N_I|_{\Omega_e} \in \mathcal{P}_k(\Omega_e)\}, \qquad I = 1, \ldots, M \tag{11}$$

where M denotes the number of nodes in the mesh and $\mathcal{P}_k(\Omega_e)$ is the space of complete polynomials with the order less than or equal to k defined over element Ω_e. For the sake of brevity, we denote the set of element interiors by $\widetilde{\Omega}$ and the set of all interior edges by $\widetilde{\Gamma}$. In two dimensions, $\widetilde{\Gamma}$ refers only to those element edges that are shared by two spatially adjacent elements, and does not include edges along the physical boundary $\partial\Omega$.

The finite-element formulation we propose to approximate the solution of the gradient flow (7) is stated as: Find $\phi_h \in \mathcal{V}^h$ such that, for all $w_h \in \mathcal{W}^h$,

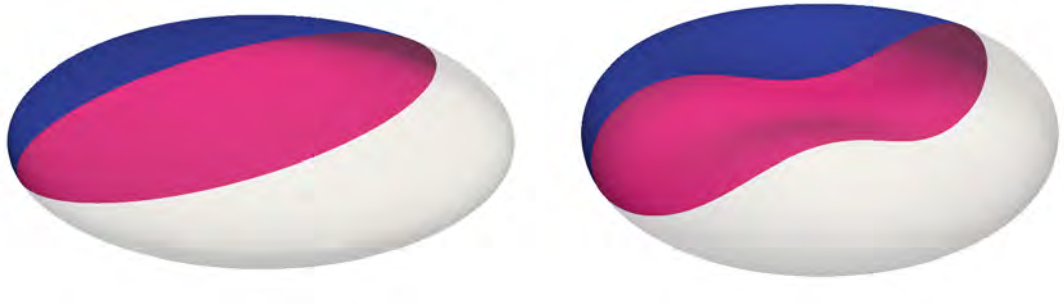
$$\begin{aligned}
\int_\Omega w_h \frac{\partial \phi_h}{\partial t}\,\mathrm{d}v = {} & \epsilon \int_{\widetilde{\Omega}} \Delta w_h \Delta \phi_h \,\mathrm{d}v + \frac{2}{\epsilon}\int_{\widetilde{\Omega}} (\nabla w_h \cdot \nabla \phi_h)(3\phi_h^2 + 2C\epsilon\phi_h - 1)\,\mathrm{d}v \\
& + \frac{1}{\epsilon}\int_{\widetilde{\Omega}} w_h(6\phi_h + 2C\epsilon)(\nabla\phi_h \cdot \nabla\phi_h)\,\mathrm{d}v \\
& + \frac{1}{\epsilon^3}\int_{\widetilde{\Omega}} w_h(3\phi_h^2 + 2C\epsilon\phi_h - 1)(\phi_h^2 - 1)(\phi_h + C\epsilon)\,\mathrm{d}v \\
& - \epsilon\int_{\widetilde{\Gamma}} [\![\nabla w_h \cdot \mathbf{n}]\!] \langle\!\langle \Delta\phi_h \rangle\!\rangle \,\mathrm{d}s - \epsilon \int_{\widetilde{\Gamma}} [\![\nabla\phi_h \cdot \mathbf{n}]\!] \langle\!\langle \Delta w_h \rangle\!\rangle \,\mathrm{d}s \\
& + \tau \int_{\widetilde{\Gamma}} [\![\nabla w_h \cdot \mathbf{n}]\!] [\![\nabla\phi_h \cdot \mathbf{n}]\!] \,\mathrm{d}s \\
& + \alpha_a \int_{\widetilde{\Omega}} w_h(A(\phi_h) - A_0)\left[-\frac{3}{2\sqrt{2}}\epsilon\left(\Delta\phi_h - \frac{1}{\epsilon^2}(\phi_h^2 - 1)\phi_h\right)\right]\,\mathrm{d}v \\
& + \alpha_v \int_{\widetilde{\Omega}} w(V(\phi_h) - V_0)\,\mathrm{d}v
\end{aligned} \tag{12}$$

where τ is the stabilization parameter which is inversely proportional to the mesh size h, i.e., $\tau \sim 1/h$ and $[\![\,\cdot\,]\!]$ and $\langle\!\langle\,\cdot\,\rangle\!\rangle$ represent the jump and average operators on element

interiors, respectively. In comparison to (9), additional terms are included in the fourth and fifth lines to weakly impose continuity of the first derivatives to the normal direction at element interior edges.

4 NUMERICAL STUDY

The finite-element formulation (12) is implemented in Multi-Physics Object Oriented Simulation Environment (MOOSE), which is an open source finite-element tool to solve partial differential equations [23]. For the implementation of (12), we use DG kernel with the standard Lagrangian shape functions and the iterative Jacobian free Newton Krylov (JFNK) method as a nonlinear solver in MOOSE. Notice that the use of the iterative Krylov subspace method enables good scalability of large simulations in parallel environment, while providing quadratic convergence without the incorporation of the exact Jacobian. In the present study, we consider an axisymmetric shape deformation of a vesicle in two dimensions.



(a) Initial shape (b) Equilibirum shape

Figure 1: The bi-concave shape example.

We consider a bi-concave shape as an initial shape of a vesicle. We choose ϵ depending on the mesh size, i.e., $\epsilon = 4h$ with h being the mesh size, to ensure enough resolution within the transition layer. We take the time step $\Delta t = 0.0001$ and the penalty parameters of $\alpha_v = 1000$ and $\alpha_a = 500$ for volume and area constraints. In MOOSE, a `QUAD8` element is used as a C^0-basis function. The stabilization parameter is chosen as proportional to $1/h$, i.e., $\tau \sim 1/h$.

Axisymmetric equilibrium vesicle shapes are determined for different values of reduced volume [24] which is the key control parameter. Figure 1(b) shows a bi-concave disc, similar in shape to a human red blood cell, obtained from the initial configuration of an oblate spheroid with a reduced volume of 0.62. As shown in Figure 2, the curvature energy decreases until a steady state is reached, indicating the shape equilibrium of the vesicle. The errors of the area and volume constraints are less than 1.5% and 2.0%, respectively.

In Figure 3, we test various types of C^0-elements using `QUAD9`, `QUAD8` and `TRI6` that are

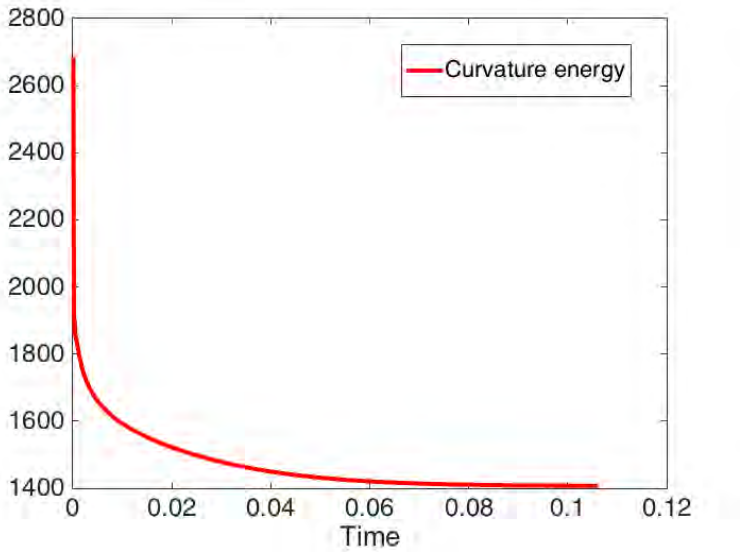
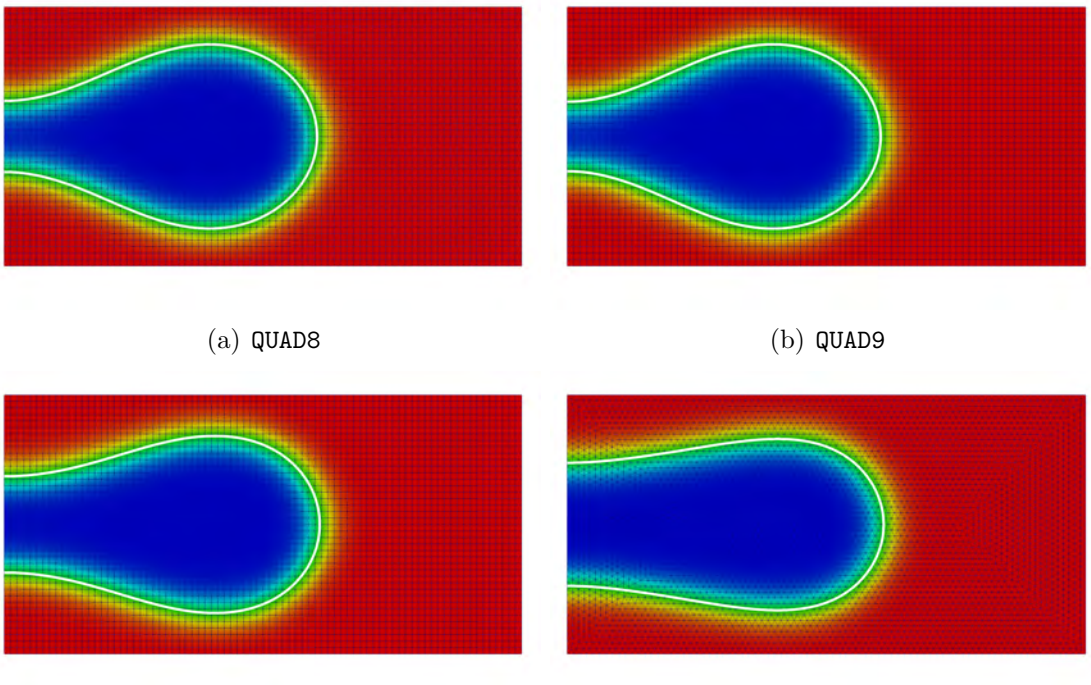


Figure 2: The evolution of curvature energy.



(a) `QUAD8` (b) `QUAD9`

(c) `HERMITE` (d) `TRI6`

Figure 3: Equilibrium shape of Bi-concave example with different element types.

available on MOOSE along with the C^1 `HERMITE` element. All the parameters are taken to be the same. It is worth mentioning that for the `HERMITE` element, the Nitsche's terms are

Element	Nodes	Elements	Area error(%)	Volume error(%)	Total time (seconds)
HERMITE	13041	3200	2.75	3.51	1906
QUAD8	9841	3200	2.89	2.58	1826
QUAD9	13041	3200	2.54	2.87	2242
TRI6	14985	7372	3.48	4.12	1956

Table 1: Comparision of number of nodes, elements, area and volume error and simulation time for different element types.

not needed and so we use the standard Galerkin formulation (9). The simulations are run until it reaches to the steady state based on the curvature energy. The final equilibrium shapes are displayed in Figure 3. The shapes of QUAD8 and QUAD9 cases are qualitatively indistinguishable and they both have good agreement with the HERMITE case except for slight deviation of the curvature near the z-axis. The shape of TRI6 does not match other cases well and it could be due to the insufficient mesh density. It should be expected that those discrepancies will be eliminated by increasing the number of elements. Some more detailed comparison is given in Table 1. For the C^0-discontinuous Galerkin method, it seems that QUAD8 is a suitable choice in terms of the accuracy and efficiency. With same number of elements, the use of QUAD8 would have less number of nodes than QUAD9 and HERMITE and thus leads to less overall simulation time.

5 CONCLUSIONS

In this paper, we introduce C^0-elements based discontinuous Galerkin formulation for the fourth-order phase-field model to predict the equilibrium shape of a vesicle. Using MOOSE, numerical study for the two-dimensional and axisymmetric bi-concave shape verifies that the proposed formulation can capture the equilibrium shape of the vesicle. In the future, we will investigate the influence of the stabilization parameter τ and the effect of the mesh size within the transition layer on the shape deformation of the vesicle. Further study will be performed for complex morphological transformations to capture various equilibrium shapes of vesicle deformation such as budding and fission. Moreover, this study will be eventually extended to the three-dimensional vesicle shape deformation.

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