# Direct computation of two-phase icosahedral equilibria of lipid bilayer vesicles

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## Highlights

- A systematic computational framework for capturing icosahedron symmetric equilibria of Lipid Bilayer Vesicles is proposed.
- Subdivision surface finite element method and symmetry reduction method are at the core of our framework.
- Parameter spaces are explored using numerical bifurcation/continuation method.

## Abstract

Correctly formulated continuum models for lipid-bilayer membranes present a significant challenge to computational mechanics. In particular, the mid-surface behavior is that of a 2-dimensional fluid, while the membrane resists bending much like an elastic shell. Here we consider a well-known "Helfrich–Cahn–Hilliard" model for two-phase lipid-bilayer vesicles, incorporating mid-surface fluidity, curvature elasticity and a phase field. We present a systematic approach to the direct computation of vesicle configurations possessing icosahedral symmetry, which have been observed in experiment and whose mathematical existence has recently been established. We first introduce a radial-graph formulation to overcome the difficulties associated with fluidity within a conventional Lagrangian description. We use the so-called subdivision surface finite element method combined with an icosahedral-symmetric mesh. The resulting discrete equations are well-conditioned and inherit equivariance properties under a representation of the icosahedral group. We use group-theoretic methods to obtain a reduced problem that captures all icosahedral-symmetric solutions of the full problem. Finally we explore the behavior of our reduced model, varying numerous physical parameters present in the mathematical model.
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*Keywords:* Membrane mechanics; Subdivision surface finite element; Numerical continuation; Symmetry reduction

## 1. Introduction

Correctly formulated continuum models for lipid-bilayer membranes, exhibiting the properties of both fluids and solids, present a significant challenge to computational mechanics. At the molecular level, lipid molecules, each com-

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prising a hydrophilic head and a hydrophobic tail, form double layers or bilayers under sufficient concentration. The heads coalesce on the two sides of the double-layer membrane, protecting the hydrophobic tails, which point inward toward the membrane mid-surface. The apparent freedom of the molecules to drift or exchange positions within the membrane is accounted for by mid-surface fluidity in the continuum model, while the mutual attraction of the heads on each of the lateral sides of the membrane leads to bending resistance much like an elastic shell. The fluidity is captured elegantly via an Eulerian formulation, while the bending elasticity demands a Lagrangian description. However, the former is incomplete without knowledge of the current configuration, while the latter leads to grossly under-determined configurations.

In this work we consider a well-known Helfrich–Cahn–Hilliard model for two-phase lipid-bilayer vesicles, incorporating mid-surface fluidity, curvature elasticity and a phase field, cf. [1–6]. In the absence of the latter, the model reduces to the well-known Helfrich model [7]. The existence of a plethora of symmetry-breaking equilibria, bifurcating from the perfect spherical shape, has been recently established for this class of phase-field models [8]. The results include configurations possessing icosahedral symmetry, which have been observed in experiments sometimes taking on rather surprising "soccer-ball" shapes [9]. Our aim here is to directly compute such configurations via symmetry methods and numerical bifurcation/continuation techniques [10]. We point out that numerical gradient-flow techniques have been used to compute equilibria in two-phase models similar to that considered here [2,4–6]. This typically involves the addition of extra internal stiffness and damping mechanisms. Moreover, that approach constitutes a rather delicate and unsystematic procedure for obtaining specific equilibria, say, inspired by an experimentally observed configuration. Certainly a great deal of patient, trial-and-error "tweaking" is required. Here we present a systematic approach to computing any equilibria within the multitude of symmetry types uncovered in [8]. We focus here on icosahedral symmetry, while methodically exploring parameter space via numerical continuation.

The outline of the work is as follows. In Section 2 we present the potential energy formulation of our problem, obtaining the weak form of the equilibrium equations in Lagrangian form. Due to the presence of curvature elasticity, an accurate finite-element model requires a $C^1$ formulation. As such, we employ the so-called subdivision surface finite element method, cf. [11,12], which was first introduced for computer-graphics applications [13]. As pointed out in [14], the resulting discrete equations are wildly ill-conditioned—a direct consequence of mid-plane fluidity. We get around this difficulty via the approach used in [4,8,15], introducing the deformation as a radial graph over the unit sphere. This effectively eliminates the grossly under-determined mid-plane deformation, leading to a well-conditioned discretized system.

Presuming a mesh with icosahedral symmetry, we present the symmetry-reduction arguments in Section 4: The energy is invariant under a group action, implying that the discrete equilibrium equations are equivariant. We then deduce a symmetry-reduced problem, implemented via a projection operator coming from group representation theory. The reduced problem captures all solutions of the full problem having icosahedral symmetry. In Section 5 we present our numerical results for the reduced problem. We obtain a veritable catalog of two-phase equilibria for various values of the parameters—all having icosahedral symmetry and all obtained via numerical continuation. Among these are several "soccer-ball" configurations.

## 2. Formulation

We begin with the following phase-field elastic-shell *potential energy* for a vesicle, defined on the current configuration, denoted by $\Sigma$, presumed isomorphic to the unit sphere $S^2$:

$$E = \int_{\Sigma}\left( BH^2 + \sigma\left(\frac{\epsilon}{2}\|\nabla_{\Sigma}\phi\|^2 + W(\phi)\right)\right)ds - pV_{\Sigma}, \tag{1}$$

subject to the constraints,

$$\int_{\Sigma} ds = 4\pi, \tag{2a}$$

$$\int_{\Sigma}(\phi - \mu)ds = 0. \tag{2b}$$

The scalar field $\phi : \Sigma \to R$ represents the phase concentration field governing the phase transition, $\nabla_{\Sigma}\phi$ is the surface gradient on the current surface configuration $\Sigma$, $H$ denotes the mean curvature of the surface $\Sigma$, $B > 0$ is the