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Retrieving Topological Information of Implicitly Represented Diffuse Interfaces with Adaptive Finite Element Discretization

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Abstract. We consider the finite element based computation of topological quantities of implicitly represented surfaces within a diffuse interface framework. Utilizing an adaptive finite element implementation with effective gradient recovery techniques, we discuss how the Euler number can be accurately computed directly from the numerically solved phase field functions or order parameters. Numerical examples and applications to the topological analysis of point clouds are also presented.

AMS subject classifications: 65N30, 57M50, 74A50, 92C05

Key words: Diffuse interface model, phase field method, Euler number, Gauss curvature, adaptive finite element, gradient recovery.

1 Introduction

Efficient and robust numerical simulations of various interfaces have been subject to much research in many applications. Indeed, the geometric and topological properties of interfaces play important roles in many physical and biological processes. For example, in biological science, the geometric shapes of bilayer vesicle membranes have significant roles in cell functions and the signal transduction pathway [11, 30, 32, 34]. Similarly, in materials science, it is well known that material thermomechanical properties depend on the underlying micro-structures characterized by interfaces.

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In recent years, diffuse interface methods have become popular approaches to simulate and model complex interfaces appearing in various applications. A well known example is the diffuse interface description of material interfaces developed by Cahn and Hilliard [6] for phase transition problems. They are also often called phase field models in the materials science community [7]. A distinct feature of the diffuse interface or phase field approach to the modeling of interfaces is that the interfaces are implicitly represented by phase field functions or order parameters so that a single set of equations may be used as the mathematical models on and across the interfaces. There is no explicit tracking of interfaces so that the numerical simulations are also insensitive to the underlying changes of interfacial topology. In the last fifty years, there have been many works related to the various extensions of diffuse interface theory and their applications in diverse fields. Until today, researches remain active on the development of the diffuse interface models for new application problems and their effective numerical implementations, see a number of reviews on the subject [1,7,35,36]. The mathematical and numerical analysis of diffuse interface models have also received much attention, see for instance [3–5,8,16,17,19–21,25,29].

The topological changes of the interfaces can be an important issue in many applications such as the study of fusion and fission of membrane vesicles as well as the study of the microstructure evolution during material phase transitions. In recent years, it has becoming an increasingly interesting topic of research to not only perform the diffuse interface simulations but also to extract useful features of the interfaces from the simulation results, including the crucial topological properties of the interfaces. The latter often involved careful studies of the geometric images obtained from the simulations, see [27] and the references cited therein. Since the diffuse interface approach is insensitive to topological events, it is natural to ask if it is possible to directly extract topological information of the underlying interface from the diffuse interface simulations without resorting to the image reconstruction. In [14], a formula for capturing the Euler number of vesicles within the diffuse interface framework was proposed. Further simplification and analysis were carried out in [15]. The key idea behind such works is based on being able to first formulate and compute the curvatures of the interfaces within the diffuse interface framework, and to then estimate the Euler number through a post-processing of the order parameter (phase field functions) by utilizing the relation between the Euler number and the Gauss curvature given by the Gauss-Bonnet theorem. In the studies reported so far, the numerical simulations were based on Fourier spectral approximations with the spatial derivatives being evaluated via the FFT. Yet, in many engineering and scientific applications of phase field methods, other discretization methods such as finite difference and finite element method have also been widely used. This motivates our current study. We demonstrate here how the Euler number of the implicitly represented interfaces may be effectively computed within an adaptive finite element discretization. We begin with a brief description of some examples of diffuse interface models and its adaptive finite element approximations in Section 2. The diffuse interface Euler formula to be implemented is then presented, following the derivation in [14]. It has a special feature