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# An Adaptive High-Order Surface Finite Element Method for Polymeric Self-Consistent Field Theory on General Curved Surfaces

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**Abstract.** In this paper, we develop an adaptive high-order surface finite element method (FEM) incorporating spectral deferred correction method for chain contour discretization to solve polymeric self-consistent field equations on general curved surfaces. The high-order surface FEM is obtained by the high-order surface geometrical approximation and the high-order function space approximation. Numerical results demonstrate that the precision order of these methods is consistent with theoretical prediction. In order to describe the sharp interface in the strongly segregated system more accurately, an adaptive FEM equipped with a new *Log* marking strategy is proposed. The *Log* marking strategy can not only label the elements that need to be refined or coarsened, but also give the refined or coarsened times, which can make full use of the information of a posterior error estimator and improve the efficiency of the adaptive algorithm. To demonstrate the power of our approach, we investigate the self-assembled patterns of diblock copolymers on several distinct curved surfaces. Numerical results illustrate the efficiency of the proposed method, especially for strongly segregated systems with economical discretization nodes.

**AMS subject classifications**: 65M60, 65M50, 65Z05

**Key words**: Self-consistent field theory, block copolymers, adaptive high-order surface finite element method, general curved surfaces, self-assembled patterns, *Log* marking strategy.

## 1 Introduction

In recent years, microphase separation of block copolymers under various types of geometrical confinements (including Euclidean and manifold confinements) has attracted

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tremendous attention due to their industrial applications [3, 4]. Geometric constraints drastically affect the formation of ordered structures under which some traditional ordered phases of block copolymers are rearranged to form novel patterns [3–8]. Theories play an important role in understanding and predicting the phase behavior of block copolymers under geometrical confinements [9–13]. Among these theories, self-consistent field theory (SCFT) [13] is one of the most powerful tools in studying the self-assembly behaviors of inhomogeneous polymers and related soft-matter systems.

There have been a few studies done on the surface SCFT calculations, versus numerous works on computing bulk structures based on SCFT. Chantawansri et al. [11] and Vorselaars et al. [14] used the spherical harmonic method to numerically simulate the SCFT model confined on the spherical surface and in the spherical shell, respectively. The global spherical harmonic method has spectral accuracy, however, it can not extend to general curved surfaces. For computing the SCFT model on general surface, Li et al. [10, 15] proposed a method similar to the finite volume method. However, there has been no theory (numerical result) to guarantee (rigorously demonstrate) the computational precision. Besides that, Li's method can not be applied to strongly segregated systems when interaction parameter $\chi N > 25$ for diblock copolymer melt. Meanwhile, even for relatively weak interaction systems $\chi N < 25$, Li's method still requires a large number contour discretization points (more than 1000) to reduce the free-energy discrepancy about $5 \times 10^{-5}$. Precisely computing strongly segregated systems is still a challenge in the SCFT computation, especially for general surface confinement. In this work, we are devoted to developing efficient high-order numerical methods for polymer SCFT on general curved surfaces.

In the past several decades, many numerical approaches have been developed to address surface problems, including the level-set method [18], the close point method [17], and the surface FEM [19, 20, 25, 26]. In this paper, we focus on the surface FEM [1, 2]. Dziuk [19] firstly proposed a linear FEM to solve the Laplace-Beltrami equation on arbitrary surfaces. Demlow and Dziuk [20] presented an adaptive linear surface FEM, and then Demlow [21] generalized the surface FEM theory to a high-order case. Wei et al. [23] generalized the superconvergence results and several gradient recovery approaches of linear FEM from flat spaces to general curved surfaces for the Laplace-Beltrami equation with mildly structured triangular meshes. Bonito and Demlow [24] gave the new posteriori error estimates with sharper geometric error estimators for surface FEMs. After about 25 years of development, the surface FEM has been applied to a wide range of scientific problems, see recent review papers [25, 26] and references therein.

In our previous work [12], we proposed a linear surface FEM to study the microphase separation of block copolymers on general curved surfaces. However, in SCFT calculations, using the linear surface FEM to achieve a relatively high numerical precision may result in heavy computational complexity. Meanwhile, in strong segregation regime, self-assembled structures have two-scale spatial distribution: sharp interfaces and damped internal densities, making the uniform mesh method inefficient. Therefore it is necessary to improve this numerical method. The main contributions of this work include: