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High-Order BDFk Parametric Finite Element Methods for Anisotropic Surface Diffusion Flows and Applications in Solid-State Dewetting

Lechuan Gu, Yihang Guo and Meng Li*

School of Mathematics and Statistics, Zhengzhou University, Zhengzhou 450001, China.

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Abstract. In this paper, we extend the BGN formulation [J.W. Barrett, H. Garcke and R. Nürnberg, J. Comput. Phys. **222** (2007)] by incorporating the k-order backward differentiation formulae (BDFk) for time discretization. This allows us to develop high-order temporal parametric finite element methods for simulating anisotropic surface diffusion flows and solid-state dewetting problems, achieving accuracy levels from second-order to fourth-order. We prove the well-posedness of the constructed high-order schemes. The proposed schemes maintain good mesh quality characteristic of the classical first-order BGN scheme. Finally, we present several numerical simulations to demonstrate the high-order temporal accuracy and verify the preservation of good mesh quality and energy stability throughout the evolution.

AMS subject classifications: 65M60, 65M12, 53C44, 35K55

Key words: Parametric finite element method, BGN scheme, BDFk, high-order accuracy, energy stability.

1. Introduction

Surface diffusion refers to the movement of atoms, ions, molecules, and atomic clusters along the surface of a solid. The anisotropy of solid materials, characterized by varying periodicity and density of atomic arrangements in different lattice directions, leads to direction-dependent physical and chemical properties. This intrinsic anisotropy gives rise to anisotropic surface energy, which in turn governs anisotropic surface diffusion on solid surfaces [44]. Anisotropic surface diffusion is crucial in various applications across materials science and physics, including the evolution of voids in microelectronic circuits [41], microstructural evolution in solids [13,22], and solid-state dewetting (SSD) [26,36,39,40, 45,46,50], among others.

*Corresponding author. *Email addresses:* `gulechuanzzu@outlook.com` (L. Gu), `15836578103@163.com` (Y. Guo), `limeng@zzu.edu.cn` (M. Li)

Let $\Gamma = \Gamma(t)$ be a two-dimensional closed curve represented as

$$\vec{X} := \vec{X}(s,t) = \big(x(s,t), y(s,t)\big)^T,$$

where s is the arc-length parametrization of Γ and t denotes time — cf. Fig. 1. Besides, let $\vec{n} = (n_1, n_2)^T \in \mathbb{S}^1$ be the outward unit normal vector, $\gamma = \gamma(\vec{n})$ a given anisotropic surface energy, and $\vec{\tau} = \partial_s \vec{X} = \vec{n}^\perp$, $\vec{n} = -\partial_s \vec{X}^\perp = -\vec{\tau}^\perp$, where $\perp$ denotes the clockwise rotation by angle $\pi/2$.

We consider a homogeneous extension $\gamma(\vec{p}) : \mathbb{R}^2_* := \mathbb{R}^2 \setminus \{\vec{0}\} \to \mathbb{R}^+$ of the anisotropic surface energy $\gamma(\vec{n}) : \mathbb{S}^1 \to \mathbb{R}^+$ such that:

(i) $\gamma(\vec{p})|_{\vec{p}=\vec{n}} = \gamma(\vec{n})$ for $\vec{n} \in \mathbb{S}^1$,

(ii) $\gamma(c\vec{p}) = c\gamma(\vec{p})$ for $c > 0$ and $\vec{p} \in \mathbb{R}^2_*$.

One of popular homogeneous extensions is

$$\gamma(\vec{p}) := |\vec{p}|\gamma\left(\frac{\vec{p}}{|\vec{p}|}\right) \quad \text{for all} \quad \vec{p} = (p_1, p_2)^T \in \mathbb{R}^2_* := \mathbb{R}^2 \setminus \{\vec{0}\},$$
$$\gamma(\vec{p}) := 0, \vec{p} = \vec{0},$$

where $|\vec{p}| = \sqrt{p_1^2 + p_2^2}$, cf. Refs. [2,15,29].

The following geometric evolution equation

$$\partial_t \vec{X} = \partial_{ss}\mu\vec{n}, \tag{1.1}$$

where $\mu := \mu(s)$ is the chemical potential, characterizes the motion of the curve driven by anisotropic surface diffusion [14, 40, 42]. The Cahn-Hoffman $\vec{\xi}$-vector [23, 47], the

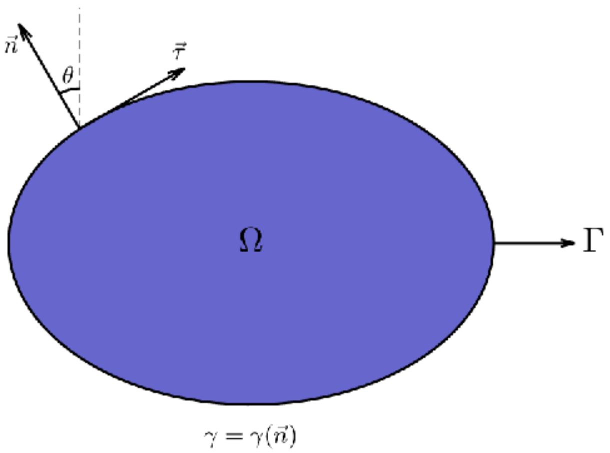

Figure 1: Schematic diagram of a closed curve Γ under anisotropic surface diffusion. The anisotropic surface energy is $\gamma(\vec{n})$, while $\vec{n}$ is the outward unit normal vector.