Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0157

Vol. **38**, No. 3, pp. 729-765
September 2025

Efficient Energy-Stable Parametric Finite Element Methods for Surface Diffusion Flow and Applications in Solid-State Dewetting

Meng Li*, Yihang Guo and Jingjiang Bi

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

Received 13 July 2024; Accepted (in revised version) 8 February 2025

Abstract. Currently existing energy-stable parametric finite element methods for surface diffusion flow and other flows are usually limited to first-order accuracy in time. Designing a high-order algorithm for geometric flows that can also be theoretically proven to be energy-stable poses a significant challenge. Motivated by the new scalar auxiliary variable approach [1], we propose novel energy-stable parametric finite element approximations for isotropic/anisotropic surface diffusion flows, achieving both first-order and second-order accuracy in time. Additionally, we apply the algorithms to simulate the solid-state dewetting of thin films. Finally, extensive numerical experiments validate the accuracy, energy stability, and efficiency of our developed numerical methods. The designed algorithms in this work exhibit strong versatility, as they can be readily extended to other high-order time discretization methods (e.g., BDFk schemes). Meanwhile, the algorithms achieve remarkable computational efficiency and maintain excellent mesh quality. More importantly, the algorithm can be theoretically proven to possess unconditional energy stability, with the energy nearly equal to the original energy.

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

Key words: Surface diffusion flow, parametric finite element method, energy-stable, solid-state dewetting, scalar auxiliary variable approach.

1 Introduction

Surface diffusion (SDF) involves the movement and migration of surface atoms, atomic clusters, and molecules on material surfaces and interfaces in solids. This phenomenon is widely studied in materials and surface science [2], and it is crucial for various processes

*Corresponding author. *Email addresses:* limeng@zzu.edu.cn (M. Li), 15836578103@163.com (Y. Guo), bijingjiang@gs.zzu.edu.cn (J. Bi)

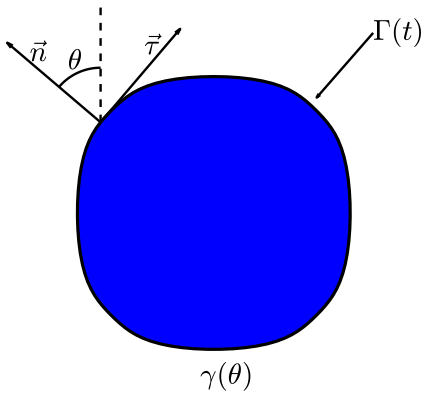

Figure 1: An illustration of SDF on a closed curve $\Gamma(t)$ with anisotropic surface energy density in two dimensions.

such as thin film growth, catalysis, epitaxial growth, and the formation of surface phases [3]. SDF can be categorized based on the orientation of the surface lattice, leading to either isotropic or anisotropic SDF. Anisotropic SDF, in particular, has extensive applications in materials science and solid-state physics, including the crystal growth of nanomaterials [4,5], morphology development in alloys, and solid-state dewetting (SSD) [6–8].

The SSD process is a significant application of SDF occurring in solid-solid-vapor systems. In these systems, the solid film adhering to the surface is often unstable or metastable in its as-deposited state, leading to complex morphological evolution driven by surface tension and capillarity effects, including edge retraction [9–11], faceting [6,12,13] and fingering instabilities [14–17]. This phenomenon, commonly observed in various thin film/substrate systems, characterized by the maintenance of the thin film in a solid state during the process [18–20], is known as SSD. Recently, SSD has found extensive applications in modern technology. For example, SSD of thin films in micro-/nanodevices can lead to the surface instabilities of well-prepared patterned structures; however, they can be leveraged for generating well-defined patterns of nanoscale particle arrays. These arrays are subsequently applied in sensors [21], optical and magnetic devices [22], as well as catalysts for the growth of carbon and semiconductor nanowire [23].

As depicted in Fig. 1, $\Gamma(t)=(x(s,t),y(s,t))^T$ denotes a closed curve in the two-dimensional space, s is the arc length parametrization of $\Gamma(t)$, $\vec{n}=(-\sin\theta,\cos\theta)^T$ represents the unit outward normal vector to the curve with $\theta\in[-\pi,\pi]$ being the angle between $\vec{n}$ and y-axis, $\vec{\tau}$ denotes the unit tangent vector, and $\gamma(\theta)$ represents the surface energy density function. From [24,25], the anisotropic surface diffusion is governed by the following partial differential equation:

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