Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2023-0315

Vol. **35**, No. 5, pp. 1263-1286
May 2024

Efficient High-Order Backward Difference Formulae for Cahn-Hilliard Equation with the Gradient Flow in $H^{-\alpha}$

Zhongqin Xue[1], Guanghui Wen[1], Zhimin Zhang[2] and Xuan Zhao[1,*]

[1] *School of Mathematics, Southeast University, Nanjing 210096, P.R. China.*
[2] *Department of Mathematics, Wayne State University, Detroit, MI 48202 USA.*

Received 25 November 2023; Accepted (in revised version) 4 February 2024

Abstract. High-order schemes enable simulating multi-time-scale problems with relatively large time step sizes for fairly accurate solutions. An unified high-order implicit BDF-q ($q=3,4,5$) scheme is developed for the Cahn-Hilliard equation with the gradient flow in $H^{-\alpha}$,$\alpha\in(0,1]$, including the classical case and its fractional variants. Introducing the discrete gradient structure, the resulting implicit BDF-q scheme is presented to satisfy the discrete energy dissipation law, which is actually compatible with the one for the classical case as the order of the fractional Laplacian α approaches 1. The L^2 norm error estimate for the BDF-q scheme is rigorously proved by developing a discrete Young-type convolution inequality to deal with the nonlinear term along with the fractional Laplacian. Further, the high-order BDF-q scheme is shown to be less time-consuming compared to the variable-step BDF-2 scheme, while the BDF-5 scheme reduces the CPU time in long-time simulation of coarsening dynamics by almost 80%. Numerical examples also demonstrate that high-order schemes are deemed appealing for long-time slow evolution, while variable-step scheme exhibits more flexibility during phase separation at initial state. In light of this, the variable-step BDF-q scheme utilizing the adaptive time-stepping strategy is implemented to capture both the rapid and slow evolutions of the solutions efficiently and accurately even in high dimensions.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07
Key words: Cahn-Hilliard equation, high-order BDF methods, discrete gradient structure, energy stability, convergence analysis.

1 Introduction

The dynamics of phase separation and pattern-forming processes is usually described by the Cahn-Hilliard model [1–4]. The corresponding free energy takes into account just lo-

*Corresponding author. *Email addresses:* zqxue@aa.seu.edu.cn, Zhongqin.Xue@tufts.edu (Z. Xue), ghwen@seu.edu.cn (G. Wen), zzhang@math.wayne.edu (Z. Zhang), xuanzhao11@seu.edu.cn (X. Zhao)

cal interaction between the particle at a certain position and its immediate neighborhood. Related numerical methods for solving the Cahn-Hilliard type equation have been discussed in [7–9,12–15]. Besides, extensions of the Cahn-Hilliard model have been widely used to simulate interfacial problems and microstructure evolution processes, such as tumor growth [16], image inpainting [17], fronts of cells invading a wound [18], and biological aggregation [19]. However, the classical Cahn-Hilliard equation is not appropriate to precisely describe the macroscopic evolution of a microscopic model system with long-range particle interactions [20]. Over the past few decades, the fractional partial differential equations providing more realistic descriptions of complex physical process associate with anomalous diffusion are studied by various numerical procedures [21–26].

In the current study, we pay attention to the numerical approximations for the two-dimensional space fractional Cahn-Hilliard (FCH) equation in [27], derived from a gradient flow in the negative order Sobolev space $H^{-\alpha}$, of the following form

$$\partial_t\Phi=-\kappa(-\Delta)^{\alpha}\mu \quad \text{with} \quad \mu=\epsilon^2(-\Delta)\Phi+F'(\Phi), \quad (\mathbf{x},t)\in\Omega\times(0,T], \tag{1.1}$$

with initial condition $\Phi(\mathbf{x},0)=\Phi_0(\mathbf{x})$. Here, the positive constant ϵ has relation to the thickness of the interface layers between different phases and $\kappa>0$ corresponds to the mobility. We take the nonlinear term $F(u):=\frac{1}{4}(u^2-1)^2$ as the double-well potential functional. We assume that $\Phi(\mathbf{x},t)$ is periodic over the problem domain $\Omega:=(0,L)^2$. The fractional Laplacian $(-\Delta)^{\alpha}$ with the order $\alpha\in(0,1]$ is defined by the Fourier decomposition

$$(-\Delta)^{\alpha}u=\sum_{m,n\in\mathbb{Z}}\lambda_{m,n}^{\alpha}\widehat{u}_{m,n}e^{i\nu(mx+ny)},$$

where $\lambda_{m,n}:=\nu^2\left(m^2+n^2\right)$, $\nu=2\pi/L$ and $\widehat{u}_{m,n}$ refer to the Fourier coefficients. For different definitions of $(-\Delta)^{\alpha}$ and discussions about the boundary behaviors of solutions to equations with fractional Laplacian we refer the reader to [28].

The underlying Ginzburg-Landau free energy $E[\Phi]$ for the space FCH equation (1.1) can be decomposed into two parts: the interfacial free energy and the chemical free energy

$$E[\Phi]=\underbrace{\int_{\Omega}\frac{\epsilon^2}{2}|\nabla\Phi|^2\,\mathrm{d}\mathbf{x}}_{\text{Interfacial energy}}+\underbrace{\int_{\Omega}F(\Phi)\,\mathrm{d}\mathbf{x}}_{\text{Chemical energy}}. \tag{1.2}$$

Similar to the classical Cahn-Hilliard equation, the space FCH equation possesses two intrinsic physical properties. One of the properties is mass conservation, ie., $\big(\Phi(t),1\big)=\big(\Phi(0),1\big)$. Meanwhile, the free energy of the space FCH equation decreases monotonically in the sense of

$$\frac{\mathrm{d}}{\mathrm{d}t}E=\left(\frac{\delta E}{\delta\Phi},\partial_t\Phi\right)=-\kappa\left\|\partial_t\Phi\right\|^2\leq 0, \quad \forall t>0, \tag{1.3}$$