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Unconditionally Energy-Dissipation- and Maximum-Bound-Principle-Preserving Scheme for the Time-Fractional Allen–Cahn Equation

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Abstract. In this paper, we propose and analyze a class of linearly implicit energy stable scheme for the nonlinear time-fractional Allen–Cahn equation with a general potential function, where the temporal and spatial derivatives are approximated by the variable-step L1 method and the central difference method, respectively. The proposed scheme is proved to be unconditionally energy-dissipation-preserving and maximum-bound-principle-preserving in discrete settings with the help of the discrete orthogonal convolution technique. Thanks to the maximum-normal boundness of numerical solution and the discrete fractional Grönwall inequality, we obtain the convergence in L^2 norm of the proposed scheme. In practical computation, we utilize the graded mesh and the adaptive mesh to simulate the time-fractional Allen–Cahn equation to capture the multi-scale behaviors and enhance computational efficiency. Extensive numerical comparisons are provided to verify the correctness and efficiency of the proposed scheme in long-time computations.

AMS subject classifications: 65M06, 65M12, 65T50, 35R11

Key words: Time-fractional Allen–Cahn equation, energy dissipation law, maximum bound principle, adaptive time-stepping, convergence.

1 Introduction

The Phase field models are widely used in fluid dynamics, materials science, and engineering [2–4, 28, 34, 37]. Recently, models incorporating nonlocal effects [1, 17–19, 29, 33, 39, 48] have attracted significant attention. The time-fractional phase field models extend these models by incorporating fractional-order derivatives to capture long-term memory

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effects and non-locality. This extension is especially valuable for studying complex phenomena in materials and biological systems, highlighting its potential for both theoretical and practical applications.

In this paper, we numerically consider the time-fractional Allen–Cahn (tFAC) equation

$$\begin{cases} \partial_t^\alpha \Phi = -\dfrac{\delta E}{\delta \Phi} \quad \text{with} \ \dfrac{\delta E}{\delta \Phi} = -\epsilon^2 \Delta \Phi - f(\Phi), & \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad 0 < t \leq T, \\ \Phi(\mathbf{x},0) = \Phi_{\text{int}}(\mathbf{x}), & \mathbf{x} \in \bar{\Omega}, \end{cases}$$

where the spatial domain $\Omega = (a,b)^d$ represents a rectangular cell in $\mathbb{R}^d$ $(d=2,3)$, and Φ denotes the phase variable, subject to periodic boundary conditions. Here, ϵ $(0<\epsilon \ll 1)$ is an interface width parameter, f is a one-variable and continuously differentiable nonlinear potential function, $\delta E/\delta \Phi$ is the variational derivative of the energy E with respect to Φ, and the symbol ∂_t^α denotes the fractional Caputo derivative of order $\alpha \in (0,1)$

$$(\partial_t^\alpha v)(t) := \int_0^t \omega_{1-\alpha}(t-s) v'(s) \mathrm{d}s \quad \text{with} \ \omega_{1-\alpha}(t) = t^{-\alpha}/\Gamma(1-\alpha),$$

where Γ denotes the Gamma function.

It is widely acknowledged that the energy dissipation law is a key property of the classical phase field model. The classic Allen–Cahn equation satisfies the following energy dissipation law

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \int_\Omega \frac{\delta E}{\delta \Phi} \partial_t \Phi \mathrm{d}\mathbf{x} = -\int_\Omega (\partial_t \Phi)^2 \mathrm{d}\mathbf{x} \leq 0, \quad t>0,$$

where

$$E[\Phi] := \int_\Omega \Big(\frac{\epsilon^2}{2} |\nabla \Phi|^2 + F(\Phi) \Big) \mathrm{d}\mathbf{x}, \quad F' = -f.$$

Notably, there are some research on the energy structure of the tFAC Allen–Cahn equation, including, but are not limited to the following types

- Tang et al. [40] demonstrated that the solution to the tFAC equation preserves the following energy stability

  $$E[\Phi(t)] \leq E[\Phi(0)], \quad t>0.$$

  Moreover, the authors pointed out that the tFAC equation manifests the maximum bound principle (MBP)

  $$\text{for all} \quad \mathbf{x} \in \bar{\Omega}: \quad |\Phi_{\text{int}}(\mathbf{x})| \leq \beta \quad \Rightarrow \quad |\Phi(\mathbf{x},t)| \leq \beta, \quad \forall t>0, \tag{1.1}$$

  under the assumption that there exists a constant $\beta > 0$ such that

  $$f(\beta) \leq 0 \leq f(-\beta).$$