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NUMERICAL ENERGY DISSIPATION FOR TIME-FRACTIONAL PHASE-FIELD EQUATIONS*

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Abstract

The numerical integration of phase-field equations is a delicate task which needs to recover at the discrete level intrinsic properties of the solution such as energy dissipation and maximum principle. Although the theory of energy dissipation for classical phase field models is well established, the corresponding theory for time-fractional phase-field models is still incomplete. In this article, we study certain nonlocal-in-time energies using the first-order stabilized semi-implicit L1 scheme. In particular, we will establish a discrete fractional energy law and a discrete weighted energy law. The extension for a $(2-\alpha)$-order L1 scalar auxiliary variable scheme will be investigated. Moreover, we demonstrate that the energy bound is preserved for the L1 schemes with nonuniform time steps. Several numerical experiments are carried to verify our theoretical analysis.

Mathematics subject classification: 65M06, 65M12, 74A50.
Key words: Time-fractional phased-field equation, Allen-Cahn equations, Cahn-Hilliard equations, Caputo fractional derivative, Energy dissipation.

1. Introduction

A fractional time derivative arises when the characteristic waiting time diverges, which models situations involving memory. In recent years, to model memory effects and subdiffusive regimes in applications such as transport theory, viscoelasticity, rheology and non-Markovian stochastic processes, there has been an increasing interest in the study of time-fractional differential equations, i.e. differential equations where the standard time derivative is replaced by a fractional one, typically a Caputo or a Riemann-Liouville derivative. It has been reported that the presence of nonlocal operators in time in the relevant governing equations may change diffusive dynamics significantly, which can better describe certain fundamental relations between the processes of interest, see, e.g. [1, 4, 6, 18, 26]. It is also noted that an intensive effort

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has been put into investigations on time fractional phase-field models. For instance, phase-field framework has been successfully employed to describe the evolution of structural damage and fatigue [3], in which the damage is described by a variable order time fractional derivative.

Seeking numerical solutions of phase field problems has attracted a lot of recent attentions. The numerical integration of phase-field equations can be a delicate task: it needs to recover at the discrete level intrinsic properties of the solution (energy diminishing, maximum principle) and the presence of small parameter $\varepsilon > 0$ (typically, the interphase length) can generate practical difficulties. Numerical analysis and computation aiming to handle this task for the classical phase field problems have attracted extensive attentions, see, e.g. [8,12,35,39] and the references therein. On the other hand, it is natural to extend the relevant discrete level intrinsic properties, i.e. the maximum principle and energy stability to handle the time-fractional phase-field equations, see, e.g. [9,21,23,24].

This work is concerned with numerical methods for time-fractional phase-field models with the Caputo time-derivative. The time-fractional phase-field equation can be written in the form of

$$\partial_t^\alpha \phi = \gamma \mathcal{G}\mu, \tag{1.1a}$$

where $\alpha \in (0,1), \gamma > 0$ is the mobility constant, $\mathcal{G}$ is a nonpositive operator, and ∂_t^α is the Caputo fractional derivative defined by

$$\partial_t^\alpha \phi(t) \coloneqq \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\phi'(s)}{(t-s)^\alpha}\, \mathrm{d}s, \quad t \in (0,T) \tag{1.1b}$$

with $\Gamma(\cdot)$ the gamma function. Choosing different $\mathcal{G}$ and μ, one derives different phase-field models, such as the Allen-Cahn (AC) model and the Cahn-Hilliard (CH) model. In the AC model and the CH model, $\mathcal{G}$ is taken to be -1 and Δ, respectively, while in both cases μ takes the same form

$$\mu = -\varepsilon^2 \Delta\phi + F'(\phi), \tag{1.2}$$

where $\varepsilon > 0$ is the interface width parameter and F is a double-well potential functional, commonly chosen as $F(\phi) = (1-\phi^2)^2/4$ so that $F'(\phi) = \phi^3 - \phi$. Moreover, the molecular-beam epitaxy (MBE) model has two forms, with or without slope selection [43], where

$$\mathcal{G} = -1, \quad \mu = \varepsilon^2 \Delta^2 \phi + \nabla \cdot \mathbf{f}_{\mathrm{m}}(\nabla\phi) \tag{1.3a}$$

with

$$\mathbf{f}_{\mathrm{m}}(\nabla\phi) = \begin{cases} \nabla\phi - |\nabla\phi|^2 \nabla\phi & \text{with slope selection,} \\ \dfrac{\nabla\phi}{1+|\nabla\phi|^2} & \text{without slope selection.} \end{cases} \tag{1.3b}$$

For sake of simplicity, we consider the periodic boundary condition for above time-fractional phase-field problems.

The classical energy for the standard Allen-Cahn or Cahn-Hilliard equation (i.e. (1.2) with $\alpha = 1$) is

$$E(\phi) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla\phi|^2 + F(\phi) \right) \mathrm{d}x, \tag{1.4}$$

while for the MBE equation (1.3) is given by

$$E(\phi) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\Delta\phi|^2 + F_{\mathrm{m}}(\nabla\phi) \right) \mathrm{d}x \tag{1.5a}$$