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A Maximum Bound Principle-Preserving Integrating Factor BDF2 Scheme with Its Linear Iteration Algorithm for the Allen-Cahn Equation

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Abstract. The maximum bound principle (MBP) is an essential tool in understanding the key physical properties of parabolic partial differential equations. In this paper, we develop and analyze a novel, MBP-preserving, second-order nonuniform scheme for the Allen-Cahn model with general potential, namely, the integrating factor BDF2 scheme. Specifically, we employ the MBP-preserving iteration and an enhanced kernel recombination technique to show that the integrating factor BDF2 scheme preserves the MBP under a mild time-step condition and a time-step ratio condition. It is worth noting that the integrating factor approach enables the time-step condition to be decoupled from the spatial step size, thus circumventing the stringent parabolic Courant-Friedrichs-Lewy condition $\tau = \mathscr{O}(h^2)$. Additionally, the MBP-preserving iteration technique leads to an efficient and convergent linear iterative algorithm for this nonlinear scheme. We provide error estimates in the maximum norm for nonuniform time meshes without requiring global Lipschitz continuity of the potential function. Lastly, we conduct thorough numerical experiments to verify the efficacy and performance of the proposed scheme.

AMS subject classifications: 65M06, 65M12, 65M70

Key words: Allen-Cahn equation, integrating factor method, nonuniform BDF2 scheme, maximum bound principle, error estimate.

1. Introduction

Originally developed as a phase-field model in materials science, the Allen-Cahn (AC)

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model [1] has evolved into a versatile mathematical framework for analyzing interfacial dynamics and non-equilibrium phase transformations across diverse physical systems. This study focuses on the AC model described by

$$u_t = \epsilon^2 \Delta u + f(u), \quad \mathbf{x} \in \Omega, \quad t \in (0, T], \tag{1.1}$$

where $\epsilon > 0$ represents a small parameter controlling interface width between different phases, and $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ is a spatial domain. The initial value $u(\mathbf{x}, 0) = u_0(\mathbf{x})$ and the periodic boundary is imposed on $\overline{\Omega}$.

The system's energy functional

$$E[u] := \int_\Omega \left(\epsilon^2 |\nabla u|^2/2 + F(u)\right) \mathrm{d}\mathbf{x}$$

drives the L^2 gradient flow dynamics of (1.1), where the nonlinear potential $F(u)$ satisfies $F'(u) = -f(u)$. Thus, the AC model (1.1) possesses an important physical property, namely the energy dissipation law $\mathrm{d}E/\mathrm{d}t \le 0$. Two widely studied potential functions are the logarithmic Flory-Huggins potential (for $0 < \theta < \theta_c$)

$$F(u) = \frac{\theta}{2}[(1-u)\ln(1-u) + (1+u)\ln(1+u)] - \frac{\theta_c}{2}u^2, \quad f(u) = \frac{\theta}{2}\ln\left(\frac{1-u}{1+u}\right) + \theta_c u, \tag{1.2}$$

and its idealized form, the polynomial potential

$$F(u) = \frac{1}{4}(1-u^2)^2, \quad f(u) = u - u^3. \tag{1.3}$$

Among these, the logarithmic potential offers enhanced physical fidelity. The maximum bound principle is another significant property of the AC model (1.1) under the assumption that there is a constant $\beta > 0$ such that $f(\beta) \le 0 \le f(-\beta)$. This property guarantees that solutions maintain pointwise boundedness within the range $[-\beta, \beta]$ for all temporal evolution, provided the initial data satisfies $\max_{\mathbf{x}\in\overline{\Omega}} |u_0(\mathbf{x})| \le \beta$.

In the realm of numerical computations, preserving the discrete MBP is critical to ensure physically meaningful solutions and prevent computational artifacts like overflow. In recent decades, significant advancements have been achieved in the development of MBP-preserving algorithms for AC-type equations. These include stabilized implicit-explicit schemes, Runge-Kutta-type methods, operator splitting approaches, the Lagrange multiplier method, and other related techniques [2, 6, 7, 17, 24, 25, 33, 35, 41]. In addition, the exponential integrator has also made significant breakthroughs in the construction and analysis of MBP-preserving numerical schemes. One class includes the exponential time differencing (ETD) method and its variants [9, 10, 20, 21, 27], as well as the multi-step exponential method combined with the cut-off technique [23]. Another class is the integrating factor (IF) method [16, 19, 22, 26, 40], which is also referred to as the Lawson method. The IF approach has enabled the development of high-order Runge-Kutta schemes with improved stability characteristics compared to conventional strong stability-preserving (SSP) methods [11, 38], particularly eliminating the restrictive Courant-Friedrichs-Lewy (CFL)