IMPLICIT-EXPLICIT SCHEME FOR THE ALLEN-CAHN EQUATION PRESERVES THE MAXIMUM PRINCIPLE*

Tao Tang

Department of Mathematics, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China Email: tangt@sustc.edu.cn Jiang Yang Department of Applied Mathematics, Columbia University, New York, NY 10027, USA Email: jyanghkbu@gmail.com

Abstract

It is known that the Allen-Chan equations satisfy the maximum principle. Is this true for numerical schemes? To the best of our knowledge, the state-of-art stability framework is the nonlinear energy stability which has been studied extensively for the phase field type equations. In this work, we will show that a stronger stability under the infinity norm can be established for the implicit-explicit discretization in time and central finite difference in space. In other words, this commonly used numerical method for the Allen-Cahn equation preserves the maximum principle.

Mathematics subject classification: 65GXX, 65MXX. Key words: Allen-Cahn Equations, Implicit-explicit scheme, Maximum principle, Nonlinear energy stability.

1. Introduction

This paper is concerned with the numerical approximation of the Allen-Cahn equation

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

with the initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega}, \tag{1.2}$$

and subjects to the periodic or homogeneous Neumann/Dirichlet boundary conditions, where Ω is a bounded domain in \mathbb{R}^d (d = 1, 2, 3), u represents the concentration of one of the two metallic components of the alloy, and the parameter $\epsilon > 0$ represents the inter-facial width.

Without lose of generality, we consider the commonly used double well potential which gives

$$f(u) = u^3 - u. (1.3)$$

Roughly speaking, the Allen-Cahn equation (1.1) describes regions with $u \approx -1$ and $u \approx 1$ that grow and decay at the expense of one another [1]. Define the energy function in L^2 - space

$$E(u) = \int_{\Omega} \left(\frac{1}{2} \epsilon^2 |\nabla u|^2 + F(u) \right) dx, \tag{1.4}$$

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where $F(u) = \frac{1}{4}(u^2 - 1)^2$. One of the intrinsic properties of the Allen-Cahn equation is that the energy function is decreasing with time:

$$\frac{d}{dt}E(u) \le 0, \quad \forall t > 0.$$
(1.5)

The Allen-Cahn equation was originally introduced by Allen and Cahn in [1] to describe the motion of anti-phase boundaries in crystalline solids. As the exact solutions of these phasefield models can not be found, numerical methods have played an important role in various simulations. In particular, there has been extensive numerical study for approximating various phase field models, see, e.g., the survey articles of [9, 10]. One of the important numerical aspects is about the discrete stability of the numerical schemes. For the Allen-Cahn equation, some recent stability analysis can be found in [4,6,12,14,15]. To the best of our knowledge, the existing stability analysis for the phase field models has been restricted to the energy setting, see, e.g., [2, 5, 7, 8, 11, 13], and there have no rigorous l^{∞} -stability analysis for the numerical methods.

It is known that the solutions of the Allen-Cahn equation (1.1) satisfies the maximum principle, see, e.g., [3]. The primary goal of this paper is to establish a discrete L^{∞} -stability analogue. More precisely, we will show that for the implicit-explicit discretization in time and central finite difference in space, the numerical solutions for (1.1)-(1.3) can be bounded by 1 under the condition that the initial data is bounded by 1. In other words, this commonly used numerical method for the Allen-Cahn equation preserves the maximum principle.

To demonstrate the main idea, we only consider a regular solution domain in \mathbb{R}^d (d = 1, 2, 3). Without lose generality, we only consider a unit square in 2D and a cube in 3D. We also use the central finite difference to approximate the spatial derivatives and denote D_h as the discrete matrix of the Laplace operator. It is known that the discrete matrix of the Laplace operator subjected with homogeneous Dirichlet boundary conditions in 1D is given by

$$D_{h} = \Lambda_{h} := \frac{1}{h^{2}} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}_{N \times N},$$
(1.6)

where h is the width of an 1D uniform mesh. By using the notation of the Kronecker tensor product, we can obtain the discrete matrix in 2D:

$$D_h = I \otimes \Lambda_h + \Lambda_h \otimes I, \tag{1.7}$$

where I is the $N \times N$ identity matrix. Similarly, the discrete matrix of 3D case can be represented as

$$D_h = I \otimes I \otimes \Lambda_h + I \otimes \Lambda_h \otimes I + \Lambda_h \otimes I \otimes I.$$

Independent of the dimension, it can be verified that the discrete matrix D_h satisfies the following properties:

- D_h is symmetric;
- D_h is negative semidefinite, i.e.,

$$U^T D_h U \le 0, \quad \forall U \in \mathbb{R}^N; \tag{1.8}$$