Implicit-Explicit Scheme for the Allen-Cahn Equation Preserves the Maximum Principle

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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.

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

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

with the initial condition

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

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and subjects to the periodic or homogeneous Neumann/Dirichlet boundary conditions, where Ω is a bounded domain in 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

$$f(u) = u^3 - u. \tag{1.3}$$

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

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

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:

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

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 phase-field 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 [7, 9]. 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, 11, 13, 14]. 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, 8, 12, 10], 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 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

$$D_h = \Lambda_h := \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}_{N \times N}, \tag{1.6}$$

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.,

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

- Elements of D_h satisfy

$$b_{ii} = -b < 0, \quad b \geq \max_i \sum_{j \neq i} |b_{ij}|, \ \ 1 \leq i \leq N. \tag{1.9}$$

2 The discrete maximum principle and energy stability

We first prove the following useful lemma.

Lemma 1. *Let* $B \in R^{N\times N}$ *and* $A = aI - B$*, where* $a > 0$*. If* $B = (b_{ij})$ *satisfies (1.9), then*

$$||A^{-1}||_\infty \le \frac{1}{a}. \tag{2.1}$$

Proof. We first write A in the following equivalent form:

$$A = (a+b)(I - sC), \tag{2.2}$$

where b is given by (1.9), $s = b/(a+b) < 1$, and matrix $C = (c_{ij})$ satisfies

$$c_{ii} = 0, \quad \max_i \sum_{j\neq i} |c_{ij}| = \max_i \sum_{j\neq i} \left|\frac{b_{ij}}{b}\right| \le 1, \quad 1 \le i \le N. \tag{2.3}$$

By Gershgorin's circle theorem, it can be verified that

$$||C||_\infty \le 1, \quad \rho(sC) = s\rho(C) \le s < 1, \tag{2.4}$$

where $\rho(C)$ stands for the spectral radius of the matrix C. As the inverse of $I - sC$ can be represented by the power series of sC, we have

$$\begin{aligned} ||A^{-1}||_\infty &= \left|\left|\frac{1}{a+b}\sum_{p=0}^{\infty}(sC)^p\right|\right|_\infty \le \frac{1}{a+b}\sum_{p=0}^{\infty} s^p ||C||_\infty^p \\ &\le \frac{1}{a+b}\cdot\frac{1}{1-s} = \frac{1}{a}, \end{aligned} \tag{2.5}$$

where in the last step we have used the fact that $0 < s < 1$. This completes the proof of the lemma. $\square$

The most conventional approach for solving (1.1) is to use the standard implicit-explicit scheme in time and central finite difference in space:

$$\frac{U^{n+1} - U^n}{\tau} + ((U^n)^{\cdot 3} - U^n) = \epsilon^2 D_h U^{n+1}, \tag{2.6}$$

where τ denotes the time stepsize, U^n represents the vector of numerical solution at the $t = t_n$ level, and $(U^n)^{\cdot 3} = ((U_1^n)^3, (U_2^n)^3, \cdots, (U_N^n)^3)^T$.

2.1 The maximum principle

Theorem 1. *Consider the Allen-Cahn problem (1.1)-(1.3) with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the initial value is bounded by 1, i.e.,* $\max_{\boldsymbol{x}\in\bar{\Omega}}|u_0(\boldsymbol{x})| \le 1$, *then the fully discrete scheme (2.6) is also bounded by 1 in the sense that* $||U^n||_\infty \le 1$ *for all* $n > 0$, *provided that the time stepsize satisfies* $0 < \tau \le \frac{1}{2}$.

Proof. We prove our claim by induction. Obviously, $||U^0||_\infty \le \|u_0\| \le 1$. We assume $||U^m||_\infty \le 1$ and will verify the result is true for U^{m+1}. It follows from the scheme (2.6) that

$$U^{m+1} = (I - \tau\epsilon^2 D_h)^{-1}(U^m + k(U^m - (U^m)^{.3})). \tag{2.7}$$

Using Lemma 1 gives we have

$$||(I - \tau\epsilon^2 D_h)^{-1}||_\infty \le 1. \tag{2.8}$$

Note that each element of $U^m + \tau(U^m - (U^m)^{.3})$ is of the form $g(x) = x + \tau(x - x^3)$. It can be verified that if $0 < \tau \le \frac{1}{2}$ then $g'(x) \ge 0$ for $x \in [-1, 1]$. This gives that

$$\max_{|x|\le 1} g(x) = g(1) = 1; \quad \min_{|x|\le 1} g(x) = g(-1) = -1,$$

which implies that $\|g\|_\infty = 1$. Consequently, we can conclude that

$$||U^m + \tau(U^m - (U^m)^{.3})||_\infty \le 1 \quad \text{if} \quad ||U^m||_\infty \le 1. \tag{2.9}$$

This, together with (2.7) and (2.8), gives

$$||U^{m+1}||_\infty \le ||(I - \tau\epsilon^2 D_h)^{-1}||_\infty \cdot ||U^m + \tau(U^m - (U^m)^{.3})||_\infty \le 1. \tag{2.10}$$

This completes the proof. □

2.2 The discrete energy stability

Subjected with the periodic or homogeneous Neumann/Dirichlet boundary conditions, we have

$$\begin{aligned} E(u) &= \int_\Omega \Big(\frac{1}{2}\epsilon^2|\nabla u|^2 + F(u)\Big)dx \\ &= \int_\Omega \Big(-\frac{1}{2}\epsilon^2 u\triangle u + F(u)\Big)dx, \end{aligned} \tag{2.1}$$

where $E(u)$ is defined by (1.4). The discrete energy function can be represented by the discrete Laplace operator D_h given below

$$E_h(U) = h^d\Big(-\frac{\epsilon^2}{2} U^T D_h U + \sum_{i=1}^{N} \frac{1}{4}(U_i^2 - 1)^2 \Big), \tag{2.2}$$

where d is the number of dimension.

Theorem 2. *Consider the Allen-Cahn problem (1.1)-(1.3) with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the initial value is bounded by 1, i.e.,* $\max_{\boldsymbol{x}\in\bar{\Omega}} |u_0(\boldsymbol{x})| \le 1$, *then the numerical solutions obtained by the scheme (2.6) satisfies the discrete energy decreasing property:*

$$E_h(U^{n+1}) \le E_h(U^n), \tag{2.3}$$

provided that the time stepsize satisfies $0 < \tau \le \frac{1}{2}$.

Proof. Taking the difference of the discrete energy between two consective time level gives

$$\begin{aligned} & E_h(U^{n+1}) - E_h(U^n) \\ = \ & \frac{h^d}{4} \sum_{i=1}^{N} \Big[((U_i^{n+1})^2 - 1)^2 - ((U_i^n)^2 - 1)^2 \Big] - \frac{\epsilon^2 h^d}{2} \Big((U^{n+1})^T D_h U^{n+1} - (U^n)^T D_h U^n \Big). \end{aligned} \tag{2.4}$$

Note that for all $a, b \in [-1, 1]$:

$$(b^3 - b)(a - b) + (a - b)^2 \ge \frac{1}{4}[(a^2 - 1)^2 - (b^2 - 1)^2]. \tag{2.5}$$

It follows from Theorem 1 that $||U^{n+1}||_\infty, ||U^n||_\infty \le 1$ with $0 < \tau \le \frac{1}{2}$. This fact, together with (2.4), gives

$$\begin{aligned} & E_h(U^{n+1}) - E_h(U^n) \\ \le \ & h^d \sum_{i=1}^{N} \Big[((U_i^n)^3 - U_i^n)(U_i^{n+1} - U_i^n) + (U_i^{n+1} - U_i^n)^2 \Big] \\ & \quad - \frac{\epsilon^2 h^d}{2} \Big((U^{n+1})^T D_h U^{n+1} - (U^n)^T D_h U^n \Big). \end{aligned} \tag{2.6}$$

Taking L^2 inner product for (2.6) with $(U^{n+1} - U^n)^T$ yields

$$\sum_{i=1}^{N} \Big[((U_i^n)^3 - U_i^n)(U_i^{n+1} - U_i^n) + \frac{1}{\tau}(U_i^{n+1} - U_i^n)^2 \Big] = \epsilon^2 (U^{n+1} - U^n)^T D_h U^{n+1}. \tag{2.7}$$

Since the discrete Laplace operator D_h is symmetric, we can rewrite the right-hand side of (2.7) as

$$\begin{aligned}&\epsilon^2((U^{n+1}-U^n)^T D_h U^{n+1}\\ =\ &\frac{\epsilon^2}{2}((U^{n+1})^T D_h U^{n+1}-(U^n)^T D_h U^n)+\frac{\epsilon^2}{2}((U^{n+1}-U^n)^T D_h(U^{n+1}-U^n).\end{aligned}\tag{2.8}$$

Consequently, combining (2.6)-(2.8) gives

$$E_h(U^{n+1})-E_h(U^n)-\frac{\epsilon^2 h^d}{2}(U^{n+1}-U^n)^T D_h(U^{n+1}-U^n)\leq 0.\tag{2.9}$$

Since D_h is negative semidefinite, the desired result (2.3) follows from the above inequality. □

3 Unconditionally stable implicit-explicit scheme

It is shown in the previous section that the commonly used scheme (2.6) is conditionally stable. In the following numerical section we will show that the stability condition $0<\tau\leq 1/2$ is both necessary and sufficient. To obtain an unconditionally stable implicit-explicit scheme, we can add an extra perturbation term which is consistent with the truncation error. For example, we can follow [11] to give a modified scheme:

$$\frac{U^{n+1}-U^n}{\tau}+((U^n)^{.3}-U^n)+\beta(U^{n+1}-U^n)=\epsilon^2 D_h U^{n+1},\tag{3.1}$$

where $\beta>0$ is a constant.

Theorem 3. *Consider the Allen-Cahn problem (1.1)-(1.3) with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the initial value is bounded by 1, i.e.,* $\max_{\boldsymbol{x}\in\bar{\Omega}}|u_0(\boldsymbol{x})|\leq 1$, *then the numerical solutions obtained by the scheme (3.1) satisfy* $||U^n||_\infty\leq 1$ *and* $E_h(U^{n+1})\leq E_h(U^n)$, *provided that*

$$\beta+\frac{1}{\tau}\geq 2,\tag{3.2}$$

where the discrete energy E_h is defined by (2.2). In particular when $\beta\geq 2$, the numerical scheme (3.1) is unconditionally pointwise stable and energy stable.

Proof. The proof is similar to that of Theorems 1 and 2, and will be omitted here. □

4 Numerical tests

In this section, we present some numerical experiments to verify the theoretical results obtained in the previous sections. Since our analysis is independent of dimensions, for simplicity we only

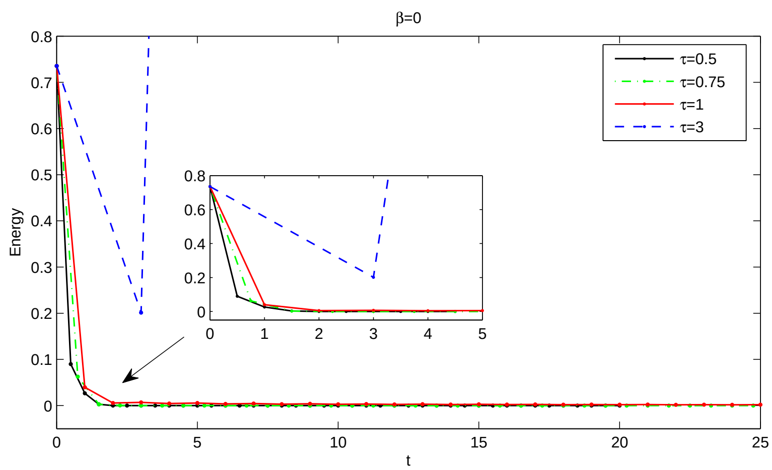

Figure 1: Energy curves for scheme (2.6) with different time steps $\tau = 0.5,\ 0.75,\ 1,\ 3$.

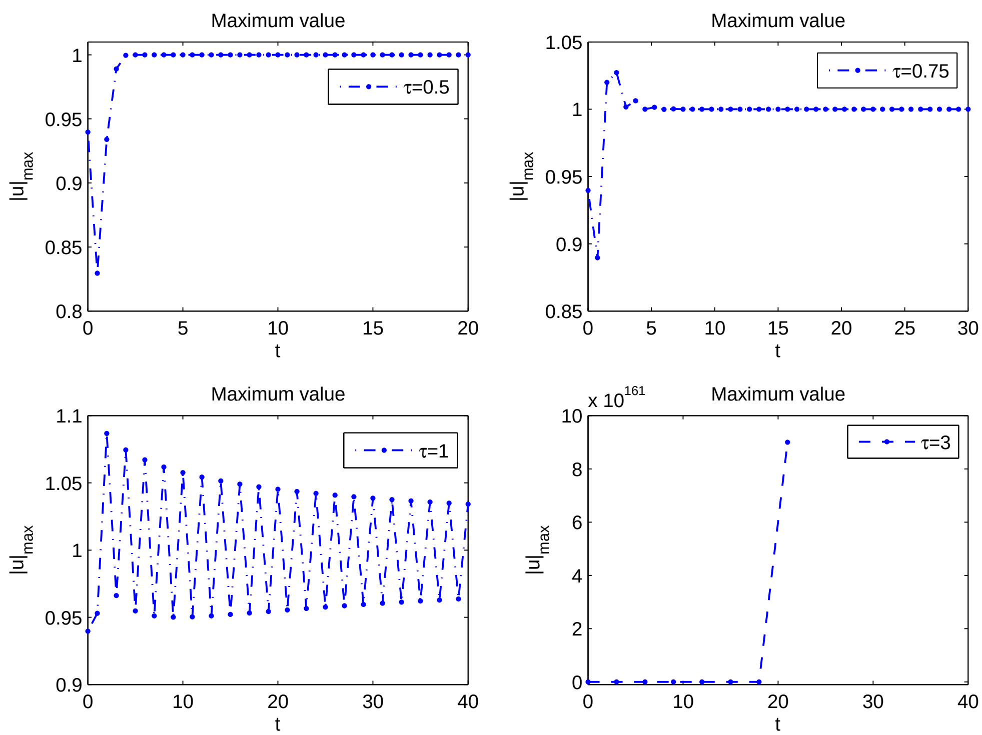

Figure 2: Maximum values for scheme (2.6) with different time steps $\tau = 0.5,\ 0.75,\ 1,\ 3$.

consider one-dimensional problems for (1.1) with homogeneous Neumann boundary condition. The initial condition is chosen as

$$u_0(x) = 0.9 \times rand(\cdot) + 0.05,$$

where "$rand(\cdot)$" represents a random number on each point in $[0, 1]$. The parameter ϵ^2 is 0.001, the computation domain is $[0, 1]$ and the mesh size in space is $h = 0.01$.

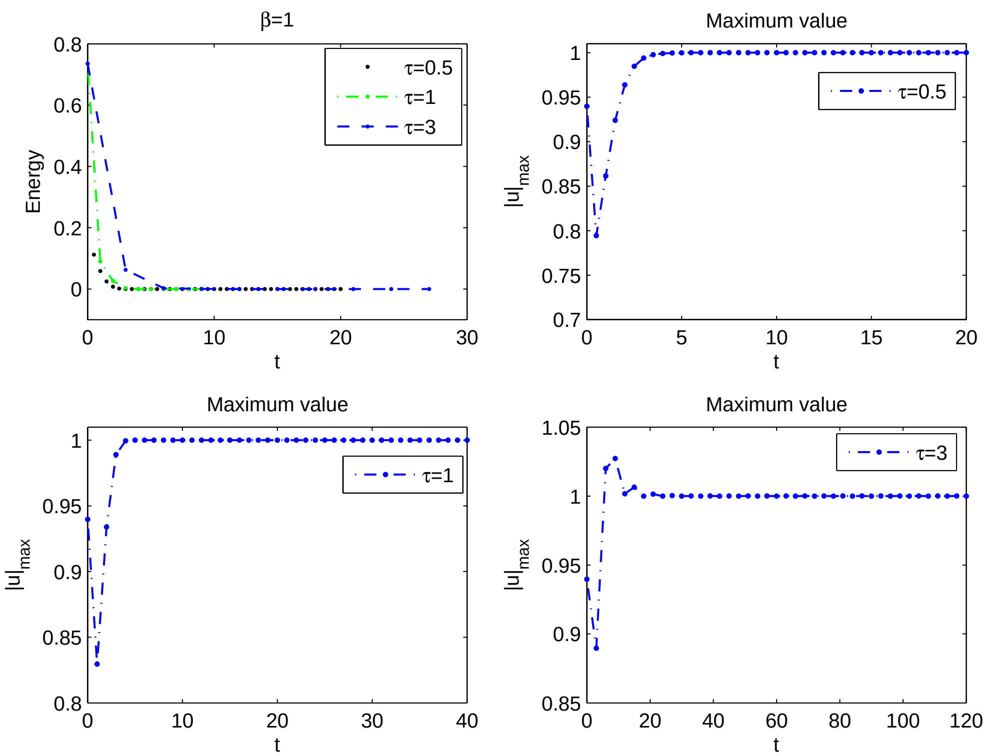

Figure 3: Energy curves and maximum values for (3.1) with $\beta = 1$ and time steps $\tau = 0.5,\ 1,\ 3$.

We first consider the standard implicit-explicit scheme (2.6). Fig. 1 plots the energy curves for several values of τ, and it is found that the energy blows up quickly when $\tau = 3$. Fig. 2 plots the maximum solution values against time, and the numerical results are in excellent agreement of our theoretical analysis. More precisely, the maximum principle is preserved for $\tau = 05$ and is violated when $\tau =\ 0.75,\ 1,\ 3$.

Fig. 3 gives the numerical results obtained using the modified scheme (3.1) with $\beta = 1$. Several time stepsizes τ are used. It is seen when the requirement $\beta + 1/\tau \geq 2$ is not satisfied with $\beta = 1$ and $\tau = 3$ the maximum principle is violated. Finally, we change β from 1 to 2 and it is observed from Fig. 4 that the corresponding scheme becomes unconditionally stable. This is in good agreement

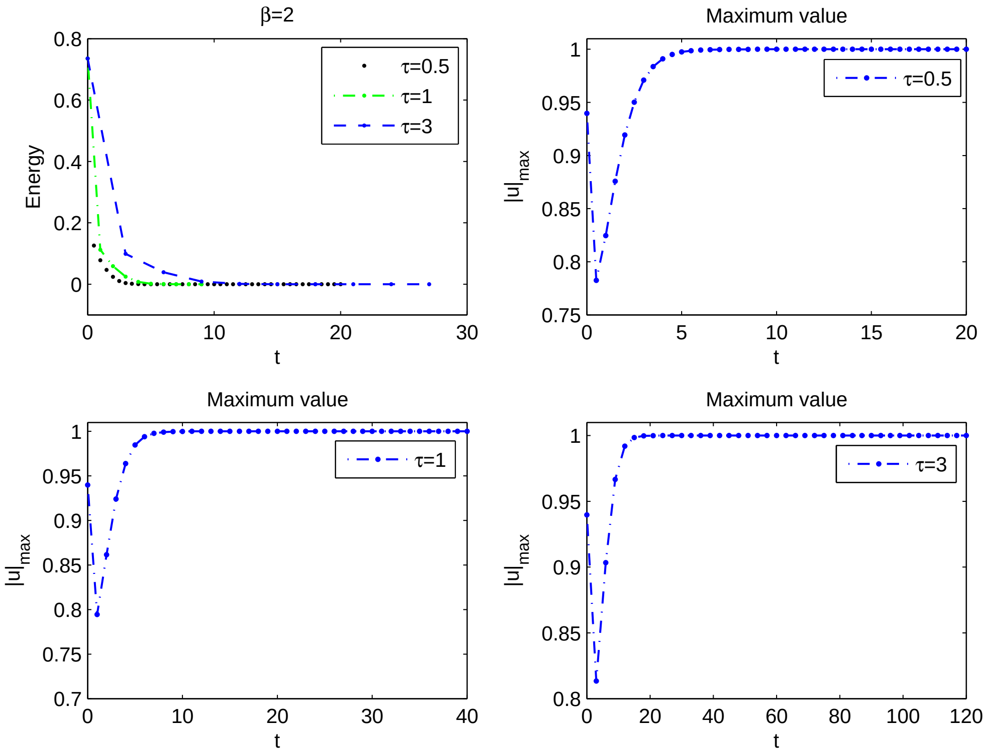

Figure 4: Same as Fig. 3, except with $\beta = 2$.

with the results of Theorem 3.

5 Concluding remarks

This works provides a theoretical framework for analyzing the l^∞-stability for the approximate solutions to the Allen-Cahn equations. Although similar theoretical results do not hold for phase field models which involve biharmonic operators, we are considering some weak version of the l^∞-stability.

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