

Numerical Analysis of the Allen-Cahn Equation with Coarse Meshes

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Dedicated to the Memory of Professor L. C. HSU on the Occasion of His 100th Birthday

Abstract In this paper, we consider the finite difference semi-discretization of the Allen-Cahn equation with the diffuse interface parameter ε . While it is natural to make the mesh size parameter h smaller than ε , it is desirable that h is as big as possible in view of computational costs. In fact, when h is bigger than ε (i.e., the mesh is relatively coarse), it is observed that the numerical solution does not move at all. The purpose of this paper is to clarify the mechanism of this phenomenon. We will prove that the numerical solution converges to that of the ordinary equation without the diffusion term if h is bigger than ε . Numerical examples are presented to support the result.

Keywords Allen-Cahn equation; finite difference method; asymptotic behavior; maximum principle

MR(2010) Subject Classification 65M06; 65M22; 35K58

1. Introduction

In this paper, we consider the Allen-Cahn equation on a bounded domain $\Omega \subset \mathbb{R}^N$:

$$\begin{cases} \partial_t u^\varepsilon - \Delta u^\varepsilon + \frac{1}{\varepsilon^2} f(u^\varepsilon) = 0, & \text{in } \Omega \times (0, T) =: Q_T, \\ \partial_n u^\varepsilon = 0, & \text{on } \partial\Omega \times (0, T), \\ u^\varepsilon|_{t=0} = u_0^\varepsilon, & \text{in } \Omega, \end{cases} \quad (1.1)$$

where $f(u) = u^3 - u$ and ∂_n denotes the normal derivative on the boundary. This is the L^2 -gradient flow of the energy functional

$$E_\varepsilon[v] = \int_\Omega \left[\frac{1}{2} |\nabla v|^2 + \frac{1}{\varepsilon^2} F(v) \right] dx, \quad (1.2)$$

where $F(u) = (1 - u^2)^2/4$. Here, $\varepsilon > 0$ is called the diffuse-interface parameter and is assumed to be small. We assume that $u_0^\varepsilon \in C^0(\overline{\Omega})$ and $\|u_0^\varepsilon\|_{L^\infty} \leq 1$. The equation (1.1) was originally proposed by Allen and Cahn [1] to describe the dynamics of antiphase boundaries in crystalline solids such as alloys, and the parameter ε describes the “width” of the interface. The equation

has been also well-studied due to its relation to the mean curvature flow (e.g., [2–5] and references therein).

Numerical analysis for the Allen-Cahn equation is widely studied for simulation of both moving interface phenomena and mean curvature flows [6–12]. In these studies, it is proved that numerical solutions converge to the solution of the Allen-Cahn equation (or the mean curvature flow) if the mesh size parameter (of the space variables) h satisfies $h = O(\varepsilon^\alpha)$ for some $\alpha > 1$. This result is natural since it is known that the diffuse interface width of the solution of (1.1) is $O(\varepsilon)$ up to the logarithmic factor [5]. Namely, the Hausdorff distance between the zero-level set of the solution of (1.1) and the solution of the mean curvature flow is $O(\varepsilon)$.

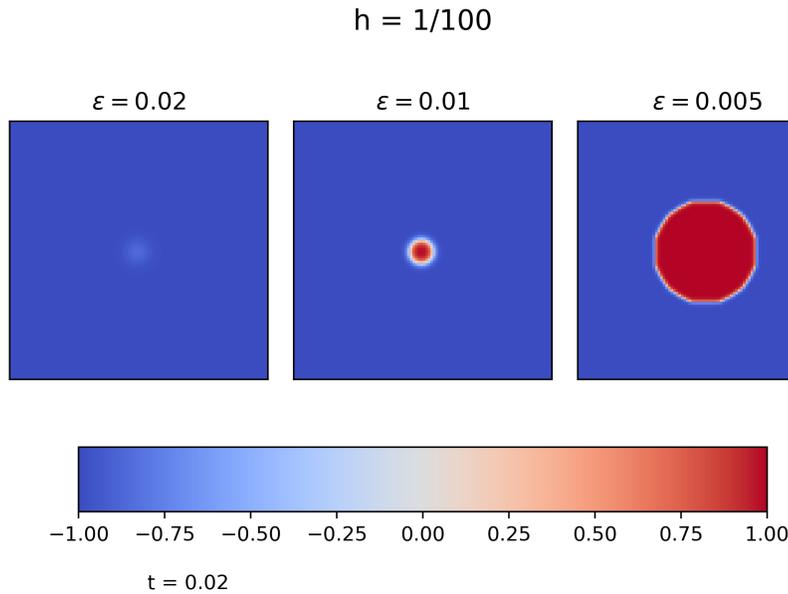


Figure 1 Snapshots at $t = 0.02$ for numerical tests with $h = 0.01$ and $\varepsilon = 0.02, 0.01, 0.005$

From the viewpoint of computational costs, however, it is desirable that h is as big as possible. One way to control computational costs is the adaptive mesh methods and many techniques are developed [13–17]. Nevertheless, we focus on the finite difference method with uniform grids, which is the simplest numerical method. In order to investigate how the (relative) magnitude of h affects numerical solutions, we show a simple numerical test. We approximated (1.1) on a domain $\Omega = (0, 1)^2 \subset \mathbb{R}^2$ by the finite difference method in space and the classical Runge-Kutta method in time, with the initial function $u_0^\varepsilon(x, y) = \tanh[d(x, y)/(\sqrt{2}\varepsilon)]$, where $d(x, y) = \sqrt{|x - 0.5|^2 + |y - 0.5|^2} - 0.2$. Then, since the sharp interface limit is the curve shortening flow whose initial curve is the circle with radius 0.2, the zero-level set of (1.1) will vanish around $t = 0.02$. We set $h = 0.01$ and computed the discrete problem for $\varepsilon = 0.02, 0.01, 0.005$. The results are shown in Figure 1. One can observe that the numerical solution for $\varepsilon = 0.02 (> h)$ is a good approximation of (1.1), the case for $\varepsilon = 0.01 (= h)$ is not bad, and the result for $\varepsilon = 0.005 (< h)$ is completely different from the exact solution. In fact, the zero-level set in

the last case is almost stationary. This result suggests that the zero-level set of the numerical solution with relatively coarse mesh (i.e., $h \gg \varepsilon$) does not move.

The purpose of the present paper is to show this conjecture for the space semi-discretization. The motion of the diffuse interface is induced by the diffusion process of the equation. Therefore, the motionless phenomenon suggests that the effect of the diffusion term is much smaller than that of the reaction term when the mesh is relatively coarse. Indeed, we will show that the numerical solution of (1.1) converges to the solution of the ordinary differential equation without the diffusion term

$$\dot{v}^\varepsilon = \frac{1}{\varepsilon^2} f(v^\varepsilon), \quad v^\varepsilon(0) = u_0^\varepsilon,$$

if $h \gg \varepsilon$ (Theorem 3.1), where the dot denotes the time derivative. This result gives a necessary condition for proper numerical computation of (1.1). The proof is based on the discrete maximum principle, which implies that the discrete Laplace operator generates a contraction semigroup (Lemma 2.1). Then, the main result will be proved by the Duhamel principle and some elementary calculation. The best possibility of the convergence rate will be discussed by numerical examples.

We mention an interesting result [18], which may be related to the present paper. In [18], finite difference approximation (with mesh size h) of the functional (1.2) and the Γ -convergence [19] of the discrete functionals are considered. Then, they proved that the Γ -limit (as $h \rightarrow 0$ and $\varepsilon \rightarrow 0$) depends on the ratio of h and ε . If $h \ll \varepsilon$, the limit is the same as that of E_ε . However, if $h \gg \varepsilon$, the limit is different and the functional Γ -converges to the so-called crystalline interfacial energy. Finally if $h \approx \varepsilon$, the Γ -limit is the interpolation of the above results. Although the subject is similar to the present study, the relation is not clear since the Γ -limit does not give the information on the corresponding gradient flows.

The organization of the rest of this paper is as follows. In Section 2, we will present some preliminary results. In particular, the discrete maximum principle will be given here. The main theorem is given in Section 3. In Section 4, numerical examples are presented to support the main result. Finally, we conclude the present paper with some remarks in Section 5.

2. Preliminaries

In what follows, we let $\Omega = (0, 1)^2 \subset \mathbb{R}^2$ be a unit square domain. Although we can consider general rectangular domains and higher dimensional cases, we let $\Omega = (0, 1)^2$ for simplicity. Let us consider the Allen-Cahn equation (1.1) in Ω for a given initial data $u_0^\varepsilon \in C^0(\bar{\Omega})$ with $\|u_0^\varepsilon\|_{L^\infty} \leq 1$. We discretize the equation in space by the finite difference method. Let $M \in \mathbb{N}$ be a positive integer and let $h = 1/M$. For a multi-index $i = (i_1, i_2) \in \mathbb{Z}^2$, we define a cell $C_i \subset \Omega$ and its center $c_i = (x_{i_1}, y_{i_2}) \in \Omega$ by

$$C_i := \left\{ (x, y) \in \Omega \mid |x - x_{i_1}| < \frac{h}{2}, |y - y_{i_2}| < \frac{h}{2} \right\} \quad x_{i_1} := \left(i_1 - \frac{1}{2} \right) h, \quad y_{i_2} := \left(i_2 - \frac{1}{2} \right) h$$

for $i \in \{1, 2, \dots, M\}^2$. Then, we define the space of piecewise constant functions $V_h \subset L^\infty(\Omega)$ by $V_h := \text{span}\{\chi_i\}_i$, where $\chi_i := \chi_{C_i}$ is the characteristic function of C_i . For a function $u_h \in V_h$,

we denote the value on a cell C_i by u_i , i.e, $u_i := u_h|_{C_i}$. Then, we define the discrete Laplace operator $\Delta_h: V_h \rightarrow V_h$ by the five-point central finite difference:

$$(\Delta_h u_h)_i := \frac{u_{(i_1-1, i_2)} + u_{(i_1+1, i_2)} + u_{(i_1, i_2-1)} + u_{(i_1, i_2+1)} - 4u_{(i_1, i_2)}}{h^2}$$

as usual. Here, we impose the discrete Neumann boundary condition for functions in V_h . That is, in the definition of Δ_h , we assume

$$u_{(i_1, 0)} = u_{(i_1, 1)}, \quad u_{(i_1, M+1)} = u_{(i_1, M)}, \quad u_{(0, i_2)} = u_{(1, i_2)}, \quad u_{(M+1, i_2)} = u_{(M, i_2)}. \tag{2.1}$$

Now, we formulate the finite difference semi-discretization of the Allen-Cahn equation (1.1) by

$$\begin{cases} \partial_t u_i^\varepsilon - \Delta_h u_i^\varepsilon + \frac{1}{\varepsilon^2} f(u_i^\varepsilon) = 0, \\ u_i^\varepsilon|_{t=0} = u_0^\varepsilon(c_i), \end{cases} \tag{2.2}$$

for all $i \in \{1, 2, \dots, M\}^2$ with the boundary condition (2.1), where $u_h^\varepsilon = \sum_i u_i^\varepsilon \chi_i \in C^1(0, T; V_h)$ is the unknown function. One can see that (2.2) is the gradient flow of the functional

$$\frac{h^2}{2} \sum_i \frac{(\delta_x^+ v_i)^2 + (\delta_x^- v_i)^2 + (\delta_y^+ v_i)^2 + (\delta_y^- v_i)^2}{2} + \frac{h^2}{\varepsilon^2} \sum_i F(v_i), \quad v_h = \sum_i v_i \chi_i \in V_h,$$

where $\delta_x^\pm v_i = \mp(v_i - v_{i\pm(1,0)})/h$ and $\delta_y^\pm v_i = \mp(v_i - v_{i\pm(0,1)})/h$. Hence the ordinary differential equation (2.2) has a smooth global solution uniquely.

We first show that the discrete Laplacian Δ_h satisfies the discrete maximum principle.

Lemma 2.1 *The semigroup $e^{t\Delta_h}$ generated by Δ_h in the topology $(V_h, \|\cdot\|_{L^\infty})$ satisfies maximum principle, that is, $v_h \geq 0 \implies e^{t\Delta_h} v_h \geq 0$ for any $v_h \in V_h$. In particular, $e^{t\Delta_h}$ is a contraction semigroup in $(V_h, \|\cdot\|_{L^\infty})$.*

Proof Let $v_h \in V_h$ and assume $v_h \geq 0$. Let moreover $w_h(t) = e^{t\Delta_h} v_h$. Then, w_h satisfies the discrete heat equation

$$\partial_t w_h = \Delta_h w_h, \quad w_h(0) = v_h. \tag{2.3}$$

We write (2.3) in matrix form as

$$\dot{\mathbf{w}}(t) = L\mathbf{w}(t), \quad \mathbf{w}(0) = \mathbf{v},$$

where $\mathbf{w}(t) \in \mathbb{R}^{M^2}$ (resp., \mathbf{v}) is the vector composed of $w_i(t)$ (resp., v_i) and $L \in \mathbb{R}^{M^2 \times M^2}$ is the matrix corresponding to the discrete Laplacian Δ_h . Then, it is clear that

$$\mathbf{w}(t) = e^{tL}\mathbf{v} = \lim_{n \rightarrow \infty} \left(I - \frac{t}{n} L \right)^{-n} \mathbf{v}. \tag{2.4}$$

Here, e^{tL} is the matrix exponential. Let $\mathbf{w}^n := (I - \tau L)^{-n} \mathbf{v}$ for $\tau > 0$. Then, \mathbf{w}^n is the solution of the backward Euler approximation of (2.3), which satisfies discrete maximum principle [20, Chanper 7]. Therefore, $v_h \geq 0$ implies $\mathbf{w}^n \geq 0$, and thus $\mathbf{w}(t) \geq 0$ from (2.4). This completes the proof. \square

We next derive the boundedness of the solution u_h^ε (see [21]).

Lemma 2.2 *Assume $\|u_0^\varepsilon\|_{L^\infty(\Omega)} \leq 1$. Then, the solution of (2.2) satisfies $\|u_h^\varepsilon(t)\|_{L^\infty(\Omega)} \leq 1$ for*

every $t \in (0, T)$.

Proof We will show $u_h^\varepsilon(t) \leq 1$. The proof of $u_h^\varepsilon(t) \geq -1$ is similar. Let

$$t_0 = \inf\{t > 0 \mid \max_i u_i^\varepsilon(t) > 1\}$$

and assume $t_0 < \infty$. We set $u_{i_0}^\varepsilon(t_0) = \max_i u_i^\varepsilon(t_0) \geq 1$. We can suppose at least one of $u_{i_0 \pm(1,0)}^\varepsilon(t_0)$ and $u_{i_0 \pm(0,1)}^\varepsilon(t_0)$ is strictly smaller than $u_{i_0}^\varepsilon(t_0)$. Then, noting that $f(u_{i_0}^\varepsilon(t_0)) \geq 0$, we have

$$\dot{u}_{i_0}^\varepsilon(t_0) = \frac{u_{i_0+(1,0)}^\varepsilon + u_{i_0+(-1,0)}^\varepsilon + u_{i_0+(0,1)}^\varepsilon + u_{i_0+(0,-1)}^\varepsilon - 4u_{i_0}^\varepsilon}{h^2} - \frac{1}{\varepsilon^2} f(u_{i_0}^\varepsilon(t_0)) < 0.$$

Therefore, from the smoothness of the solution, we can find $M > 0$ and $\delta > 0$ that satisfies

$$\dot{u}_{i_0}^\varepsilon(t) \leq -M < 0, \quad \text{if } |t - t_0| < \delta,$$

which implies

$$u_{i_0}^\varepsilon(t_0 - \delta) = u_{i_0}^\varepsilon(t_0) - \int_{t_0-\delta}^{t_0} \dot{u}_{i_0}^\varepsilon(t) dt \geq 1 + M\delta.$$

This contradicts the definition of t_0 and hence we complete the proof. \square

Next we introduce a cell-wise ordinary differential equation. Let $v_h^\varepsilon \in C^1(0, T; V_h)$ satisfy the following equation on each cell:

$$\begin{cases} \partial_t v_i^\varepsilon + \frac{1}{\varepsilon^2} f(v_i^\varepsilon) = 0, \\ v_i^\varepsilon|_{t=0} = u_0^\varepsilon(c_i), \end{cases} \tag{2.5}$$

for all $i \in \{1, 2, \dots, M\}^2$ with the boundary condition (2.1), where $v_i^\varepsilon = v_h^\varepsilon|_{C_i}$. From the general theory of dynamical systems, we have the stability of v_h^ε .

Lemma 2.3 Assume $\|u_0^\varepsilon\|_{L^\infty(\Omega)} \leq 1$. Then, the solution of (2.1) satisfies $\|v_h^\varepsilon(t)\|_{L^\infty(\Omega)} \leq 1$ for every $t \in (0, T)$.

3. Main result

We present the main result of this paper, which states that the numerical solution of the Allen-Cahn equation converges to that of the ordinary differential equation (2.5) when the mesh is relatively coarse.

Theorem 3.1 Let u_h^ε be the solution of (2.2) and v_h^ε be that of (2.5) with the same initial function u_0^ε satisfying $\|u_0^\varepsilon\|_{L^\infty(\Omega)} \leq 1$. Assume that there exists $c_0 > 0$ independently of h and ε such that

$$f'(u_0^\varepsilon(c_i)) \geq 0, \quad \forall i \in \{1, \dots, M\}^2. \tag{3.1}$$

If ε/h is sufficiently small, then we have

$$\|u_h^\varepsilon - v_h^\varepsilon\|_{L^\infty(Q_T)} \leq C\left(\frac{\varepsilon}{h}\right)^2, \tag{3.2}$$

where C depends only on c_0 .

Remark 3.2 The hypothesis (3.1) is just a technical assumption. It states that $u_0^\varepsilon(c_i) \approx \pm 1$. When the initial function u_0^ε is well-prepared [5], the relation (3.1) may hold almost surely.

Proof of Theorem 3.1 Let $w_h := u_h^\varepsilon - v_h^\varepsilon$. It is clear that $\|w_h\|_{L^\infty(Q_T)} \leq 2$ from Lemmas 2.2 and 2.3. Moreover, $w_i = w_h|_{C_i}$ satisfies $w_i(0) = 0$ and

$$\begin{aligned} \partial_t w_i &= \Delta_h w_i + \Delta_h v_i^\varepsilon - \frac{1}{\varepsilon^2} [f(w_i + v_i^\varepsilon) - f(v_i^\varepsilon)] \\ &= (\Delta_h - \alpha)w_i + \Delta_h v_i^\varepsilon + \alpha w_i - \frac{1}{\varepsilon^2} [f(w_i + v_i^\varepsilon) - f(v_i^\varepsilon)] \end{aligned}$$

for arbitrary $\alpha > 0$, with the discrete Neumann boundary condition. Thus, the Duhamel principle yields

$$w_h(t) = \int_0^t e^{(t-s)(\Delta_h - \alpha)} [\Delta_h v_h^\varepsilon(s) + G_h(s)] ds, \tag{3.3}$$

where $G_i := \alpha w_i - \varepsilon^{-2} [f(w_i + v_i^\varepsilon) - f(v_i^\varepsilon)]$ and $G_h := \sum_i G_i \chi_i$.

From the Taylor expansion, we have

$$\begin{aligned} G_i &= \left(\alpha - \frac{f'(v_i^\varepsilon)}{\varepsilon^2} \right) w_i - \frac{1}{\varepsilon^2} [f(w_i + v_i^\varepsilon) - f(v_i^\varepsilon) - f'(v_i^\varepsilon)w_i] \\ &\leq \left| \alpha - \frac{f'(v_i^\varepsilon)}{\varepsilon^2} \right| |w_i| + \frac{L}{\varepsilon^2} |w_i|^2, \end{aligned}$$

where $L = \max_{|v| \leq 2} |f''(v)|$. Moreover, let $M := \max_{|v| \leq 1} |f'(v)|$. Then, if we set $\alpha \geq M/\varepsilon^2$, we have

$$\alpha - \frac{f'(v_i^\varepsilon)}{\varepsilon^2} \geq \alpha - \frac{M}{\varepsilon^2} \geq 0.$$

On the other hand, from the assumption (3.1) and the fact that $|v_i^\varepsilon(t)| \nearrow 1$ as $t \rightarrow \infty$, we have $f'(v_i^\varepsilon(t)) = 3|v_i^\varepsilon(t)|^2 - 1 \geq c_0$ for each $t > 0$, which implies

$$\alpha - \frac{f'(v_i^\varepsilon)}{\varepsilon^2} \leq \alpha - \frac{c_0}{\varepsilon^2}.$$

Therefore, we obtain

$$|G_i| \leq \left(\alpha - \frac{c_0}{\varepsilon^2} \right) |w_i| + \frac{L}{\varepsilon^2} |w_i|^2. \tag{3.4}$$

Clearly, we have $\|\Delta_h v_h^\varepsilon\|_{L^\infty(Q_T)} \leq 8h^{-2}$. Hence, from (3.3), (3.4) and Lemma 2.1, we obtain

$$\begin{aligned} \|w_h(t)\|_{L^\infty(\Omega)} &\leq \int_0^t e^{-\alpha(t-s)} \left[\frac{8}{h^2} + \left(\alpha - \frac{c_0}{\varepsilon^2} \right) \|w_h\|_{L^\infty(Q_T)} + \frac{L}{\varepsilon^2} \|w_h\|_{L^\infty(Q_T)}^2 \right] ds \\ &\leq \frac{8}{\alpha h^2} + \left(1 - \frac{c_0}{\alpha \varepsilon^2} \right) \|w_h\|_{L^\infty(Q_T)} + \frac{L}{\alpha \varepsilon^2} \|w_h\|_{L^\infty(Q_T)}^2, \quad \forall t \in (0, T), \end{aligned}$$

which implies

$$\|w_h\|_{L^\infty(Q_T)} \leq \frac{8}{c_0} \frac{\varepsilon^2}{h^2} + \frac{L}{c_0} \frac{\varepsilon^2}{h^2} \|w_h\|_{L^\infty(Q_T)}^2.$$

Therefore,

$$\|w_h\|_{L^\infty(Q_T)} \leq A_- \quad \text{or} \quad A_+ \leq \|w_h\|_{L^\infty(Q_T)},$$

where

$$A_\pm = \frac{c_0 h^2 \pm \sqrt{c_0^2 h^4 - 32L\varepsilon^4}}{2L\varepsilon^2}.$$

We notice that A_{\pm} are well-defined as real numbers when $(\varepsilon/h)^4 \leq c_0^2/(32L)$.

Now, assume that $(\varepsilon/h)^2 < c_0/(4L)$. Then

$$A_+ \geq \frac{c_0 h^2}{2L\varepsilon^2} > 2 \geq \|w_h\|_{L^\infty(Q_T)}.$$

Hence we have

$$\|w_h\|_{L^\infty(Q_T)} \leq A_- = \frac{16\varepsilon^2}{c_0 h^2 + \sqrt{c_0^2 h^4 - 32L\varepsilon^4}} \leq \frac{16\varepsilon^2}{c_0 h^2},$$

which is the desired estimate. \square

4. Numerical examples

In this section, we present numerical examples to investigate whether the convergence rate of (3.2) is best possible. We computed (2.2) with random initial values and $T = 0.001$ for 24 pairs (h, ε) . The pair (h, ε) was selected from the set

$$\{1/20, 1/40, 1/60, 1/80, 1/100, 1/120\} \times \{0.01, 0.005, 0.002, 0.001\}.$$

We computed ten times for each (h, ε) and evaluated the L^∞ -error $\|u_h^\varepsilon - v_h^\varepsilon\|_{L^\infty(Q_T)}$. We used the classical Runge-Kutta method as a time integrator with $\Delta t = 0.1\varepsilon^{2.5}$.

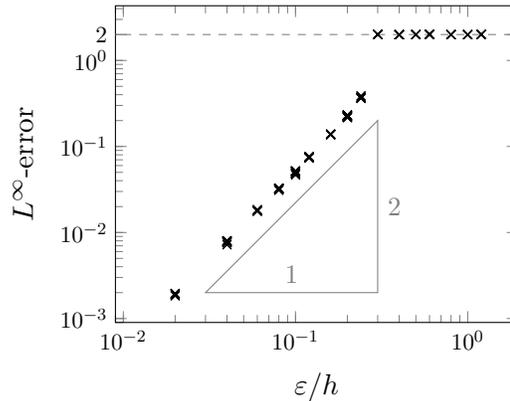


Figure 2 Behavior of L^∞ -errors with initial values satisfying (3.1)

In the first example, which is illustrated in Figure 2, we assumed that $u_i^\varepsilon(0) = v_i^\varepsilon(0) \in [-1, -0.5] \cup [0.5, 1]$ so that the assumption (3.1) is satisfied. We plotted $\|u_h^\varepsilon - v_h^\varepsilon\|_{L^\infty(Q_T)}$ for each numerical results in Figure 2, that is, ten marks are plotted for each pair (h, ε) . One can observe that the numerical solution u_h^ε is close to v_h^ε when $\varepsilon/h < 0.3$, and that the convergence rate is $O((\varepsilon/h)^2)$. Thus the estimate (3.2) may be best possible.

We also show a numerical example that does not satisfy the assumption (3.1). We computed the same problem with random initial values $u_i^\varepsilon(0) = v_i^\varepsilon(0) \in [-1, -0.1] \cup [0.1, 1]$, which do not fulfill (3.1). The result is illustrated in Figure 3. Although the variance becomes bigger than the previous example, the convergence rate seems the same as above. Thus we may make the hypothesis of Theorem 3.1 weaker.

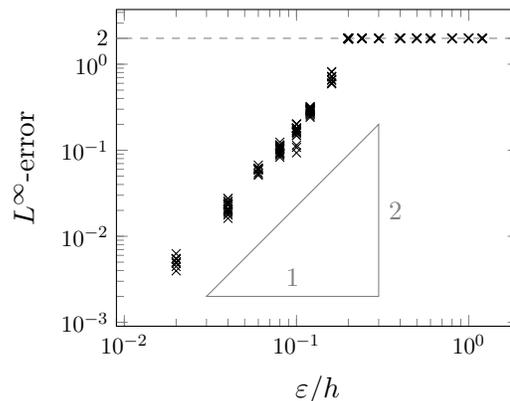


Figure 3 Behavior of L^∞ -errors with initial values without (3.1)

5. Concluding remarks

In this paper, we studied the behavior of semi-discretized solution of the Allen-Cahn equation for relatively coarse meshes. The main statement of the present paper is that the numerical solution converges to that of an ordinary differential equation without the diffusion term (Theorem 3). From the model, it is of course clear that the numerical computation does not succeed when the mesh size h is bigger than ε . However, our contributions are that we proposed a necessary condition for accurate numerical computation and that we identified the mechanism of the failure of numerical simulation.

We imposed a technical assumption (3.1) for the main result. Although it is essential in our proof, the numerical example suggests that it may be unnecessary. The proof is also based on the discrete maximum principle (Lemma 2.1). Therefore, it is not clear whether the same result holds for the finite element approximation. However, for the finite element method with mass-lumping technique, the discrete maximum principle holds for Delaunay type triangulation [22, Theorem 5.1], and thus our result can be extended.

We addressed only semi-discretization of the Allen-Cahn equation. Obviously, it is the most important to investigate fully discretized solution. Furthermore, the behavior of the numerical solution for $h \approx \varepsilon$ is not trivial. In that case, it is expected that the behavior may be interpolation of the Allen-Cahn equation and the ordinary differential equation. We will investigate such problems in future work.

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